



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 08:53 PM JST

PDB ID : 8Y5K / pdb\_00008y5k  
EMDB ID : EMD-38940  
Title : E.coli transcription translation coupling complex in TTC-A state 2 containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin  
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.  
Deposited on : 2024-01-31  
Resolution : 6.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

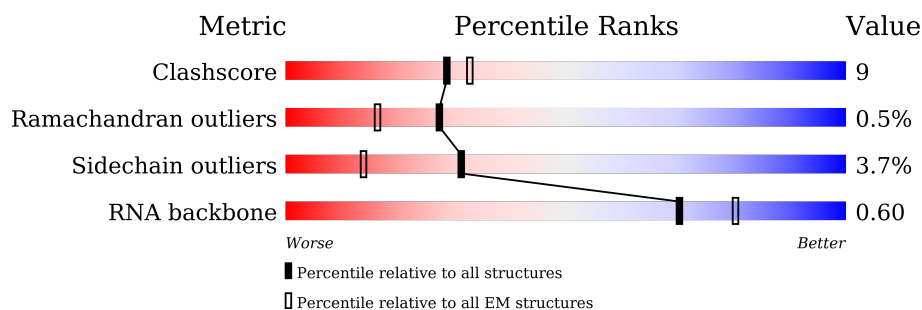
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	70	 64% 29% 6%
2	B	57	 79% 19%
3	C	55	 75% 16% 9%
4	D	46	 67% 30%
5	E	65	 77% 22%
6	F	38	 71% 29%
7	G	241	 70% 18% 10%



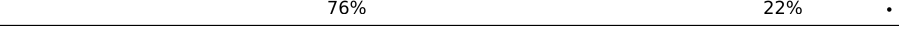
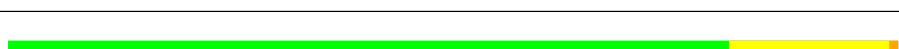



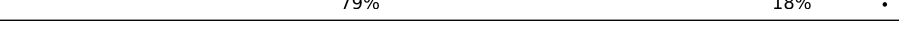



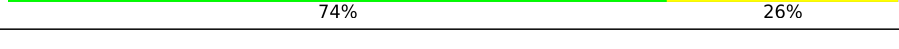

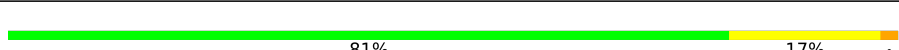


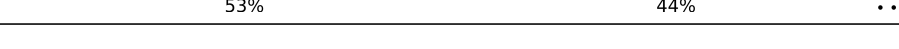
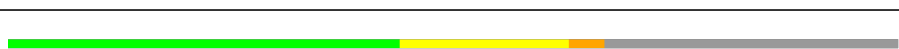
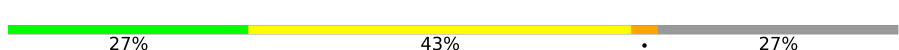
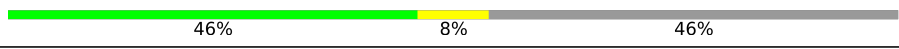




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Mol	Chain	Length	Quality of chain
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	
27	b	273	
28	c	209	
29	d	201	
30	e	179	
31	f	177	
32	g	149	






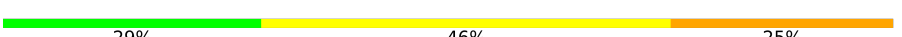




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Mol	Chain	Length	Quality of chain
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	
54	4	27	
55	8	37	
56	9	37	
57	A1	329	

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Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NG	181	
62	5	76	
63	6	77	
64	a	234	
65	0	716	
66	h	6	

## 2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 179757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 3 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	206	Total	C	N	O	S	0	0
			1620	1025	304	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total	C	N	O	S	0	0
			1152	717	218	211	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	u	102	Total	C	N	O	0	0
			776	489	146	141		

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1929590828

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	U	conflict	GB NR_103249

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	18	Total	C	N	O	P	0	0
			387	172	67	130	18		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		
57	A2	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10496	6580	1833	2040	43		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NG	88	Total	C	N	O	0	0
			433	257	88	88		

- Molecule 62 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 63 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 64 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 65 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	0	697	Total	C	N	O	S	0	0
			5399	3403	929	1042	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

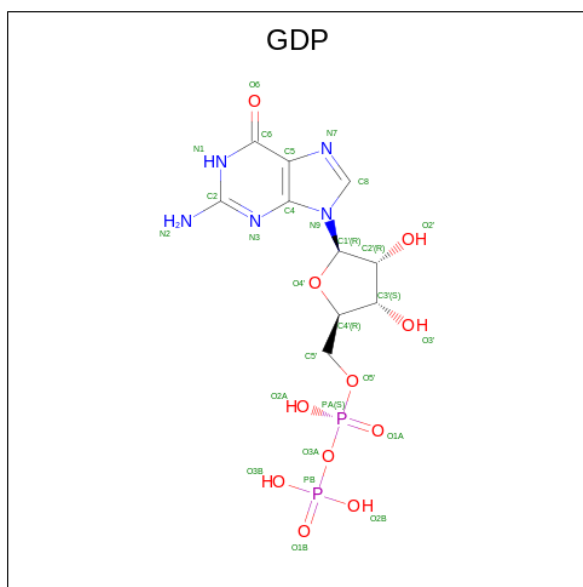
- Molecule 66 is a protein (with D amino acids) called Viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	B1	1	Total	Mg	0
			1	1	

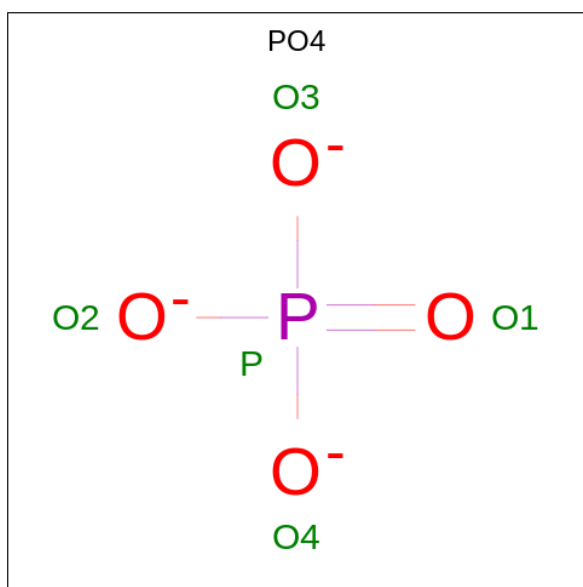
- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
68	0	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 69 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
69	0	1	5	4	1	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L31

Chain A: 



- Molecule 2: 50S ribosomal protein L32

Chain B: 



- Molecule 3: 50S ribosomal protein L33

Chain C: 




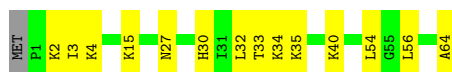
- Molecule 4: 50S ribosomal protein L34

Chain D: 



- Molecule 5: 50S ribosomal protein L35

Chain E: 



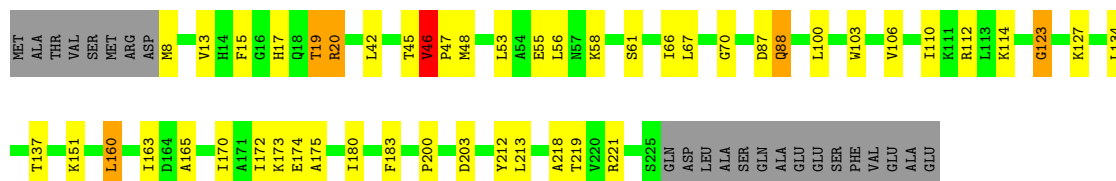
- Molecule 6: 50S ribosomal protein L36

Chain F:  71% 29%



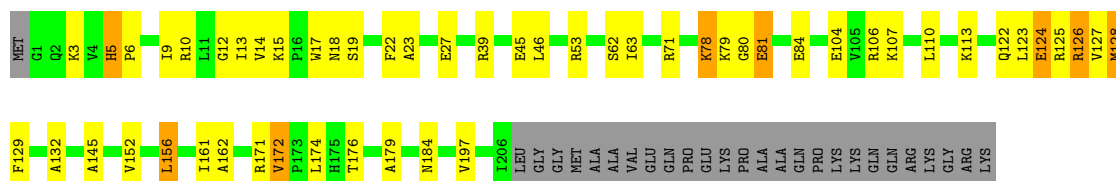
- Molecule 7: 30S ribosomal protein S2

Chain G:  70% 18% 10%



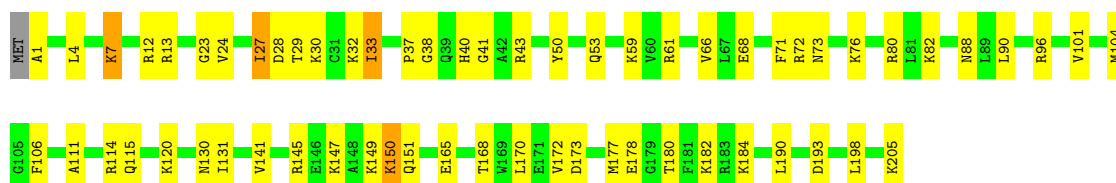
- Molecule 8: 30S ribosomal protein S3

Chain H:  66% 19% 12%



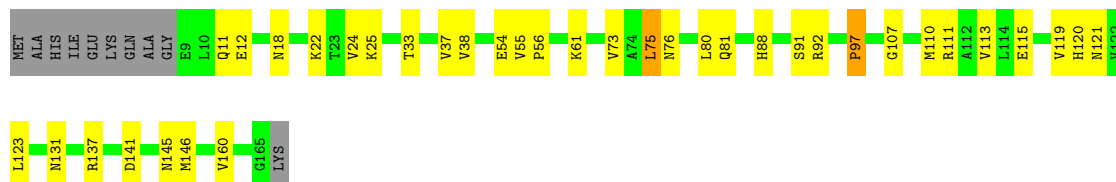
- Molecule 9: 30S ribosomal protein S4

Chain I:  69% 28%



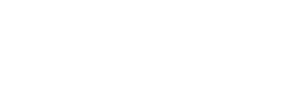
- Molecule 10: 30S ribosomal protein S5

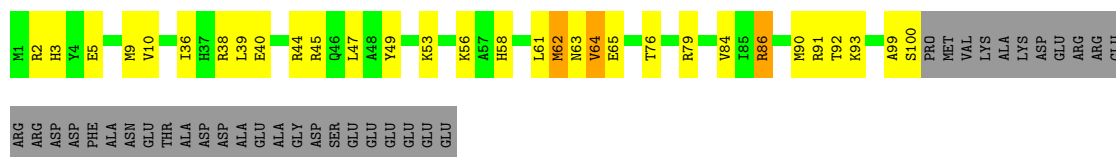
Chain J:  72% 21% 6%



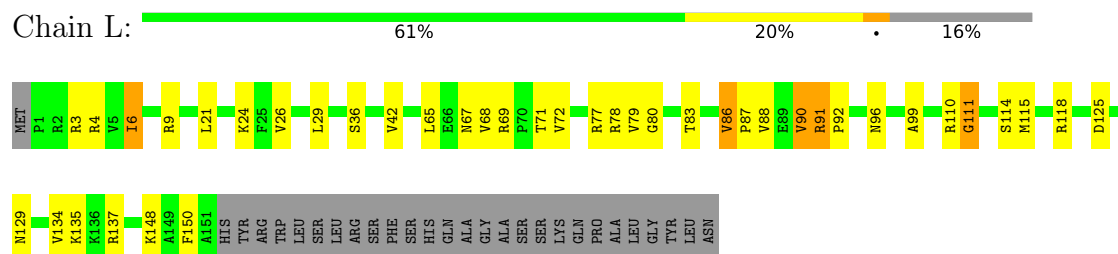
- Molecule 11: 30S ribosomal protein S6, fully modified isoform

Chain K:  51% 21% 26%

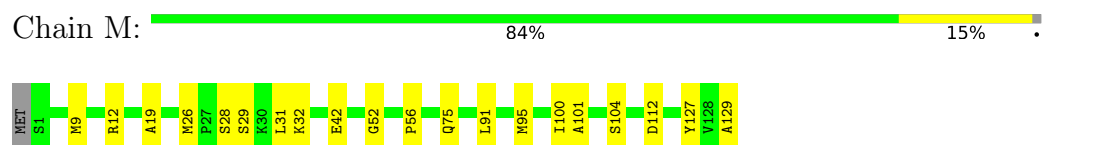




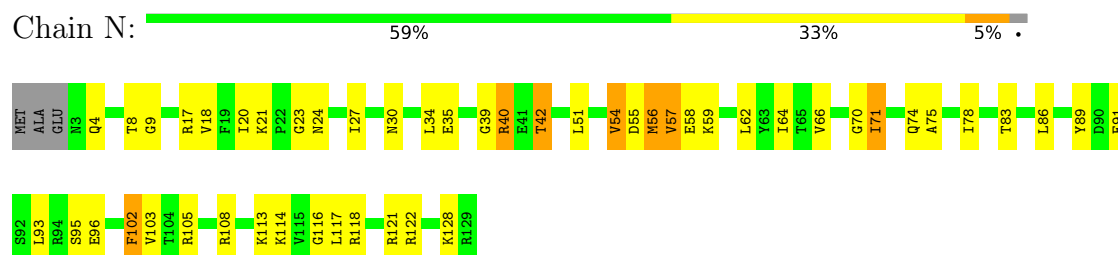
• Molecule 12: 30S ribosomal protein S7



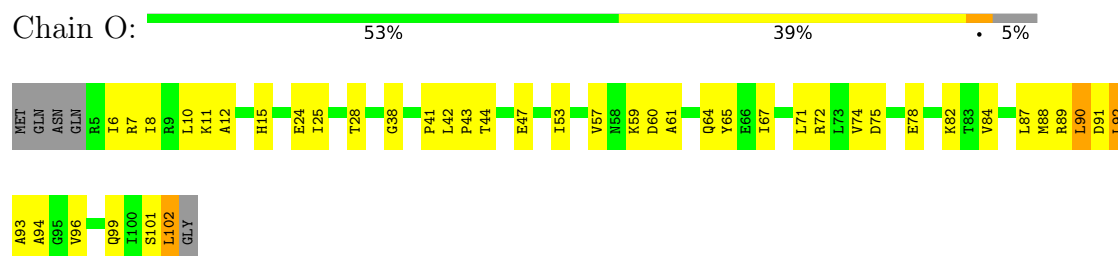
• Molecule 13: 30S ribosomal protein S8



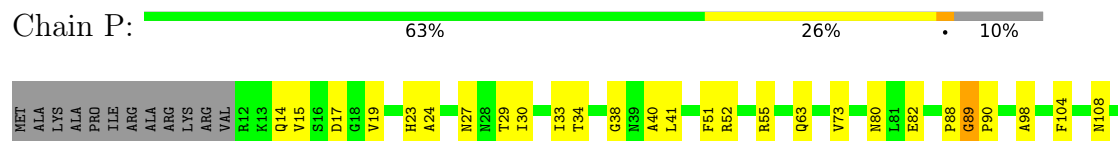
• Molecule 14: 30S ribosomal protein S9



• Molecule 15: 30S ribosomal protein S10



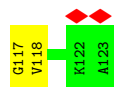
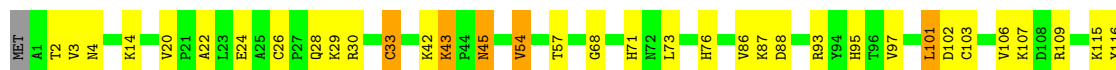
• Molecule 16: 30S ribosomal protein S11





- Molecule 17: 30S ribosomal protein S12

Chain Q: 69% 26%



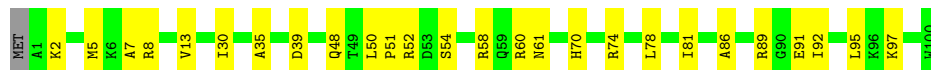
- Molecule 18: 30S ribosomal protein S13

Chain R: 72% 24%



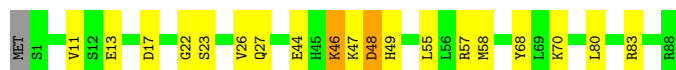
- Molecule 19: 30S ribosomal protein S14

Chain S: 73% 26%



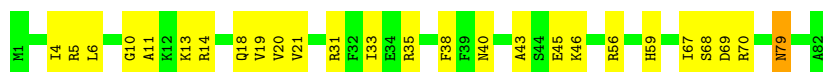
- Molecule 20: 30S ribosomal protein S15

Chain T: 78% 19%



- Molecule 21: 30S ribosomal protein S16

Chain U: 68% 30%



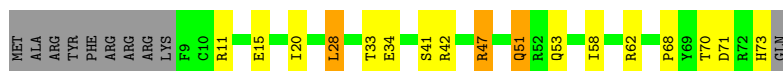
- Molecule 22: 30S ribosomal protein S17

Chain V: 61% 35% 5%



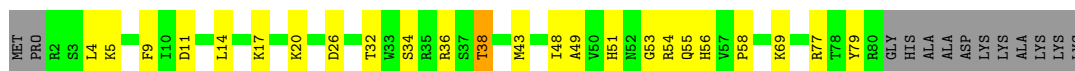
- Molecule 23: 30S ribosomal protein S18

Chain W:  64% 19% 13%



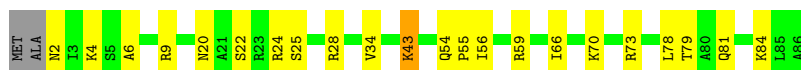
- Molecule 24: 30S ribosomal protein S19

Chain X:  60% 25% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  72% 24% ..



- Molecule 26: 30S ribosomal protein S21

Chain Z:  70% 18% 8%



- Molecule 27: 50S ribosomal protein L2

Chain b:  71% 27% ..

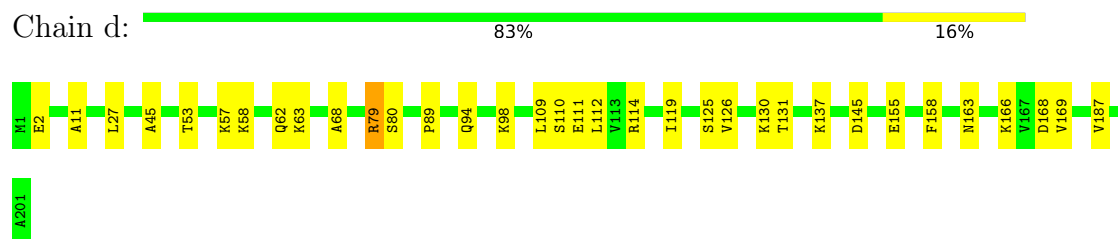


- Molecule 28: 50S ribosomal protein L3

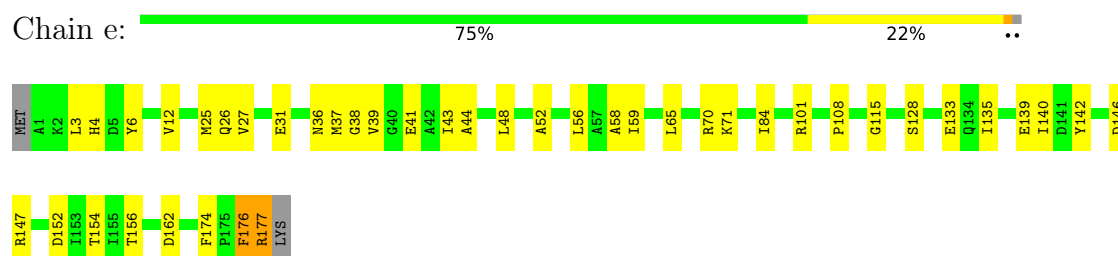
Chain c:  78% 22%



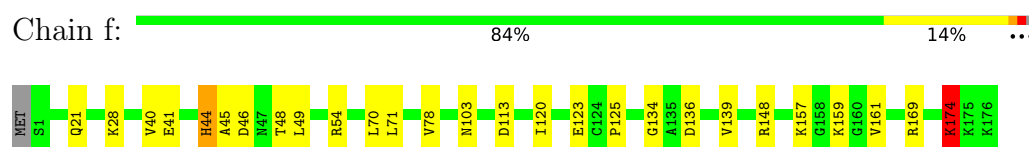
- Molecule 29: 50S ribosomal protein L4



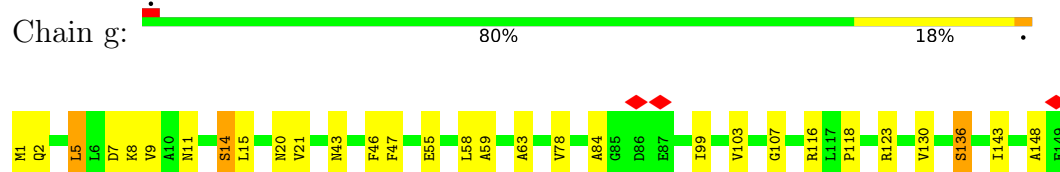
- Molecule 30: 50S ribosomal protein L5



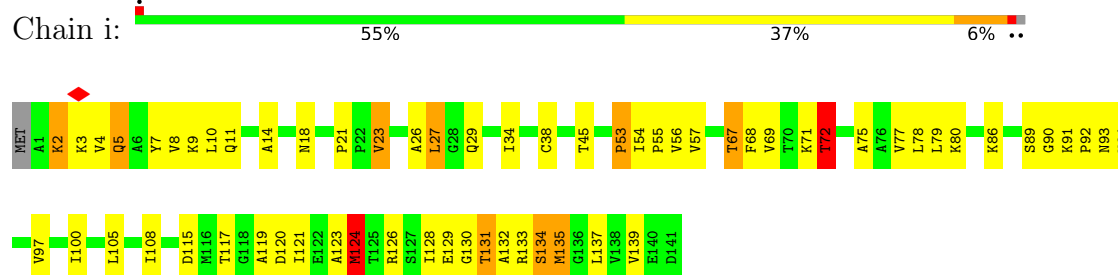
- Molecule 31: 50S ribosomal protein L6



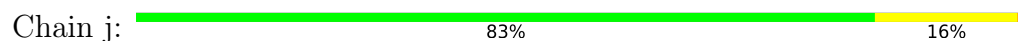
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L11



- Molecule 34: 50S ribosomal protein L13





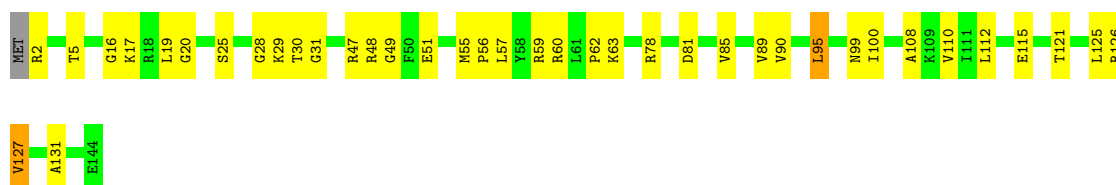
- Molecule 35: 50S ribosomal protein L14

Chain k: 76% 22% ..



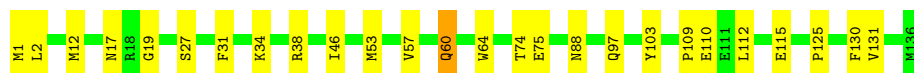
- Molecule 36: 50S ribosomal protein L15

Chain l: 72% 26% ..



- Molecule 37: 50S ribosomal protein L16

Chain m: 81% 18% .



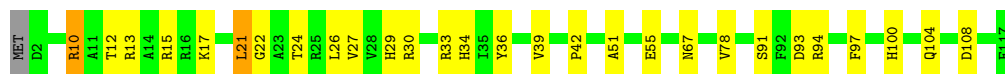
- Molecule 38: 50S ribosomal protein L17

Chain n: 75% 19% 6%



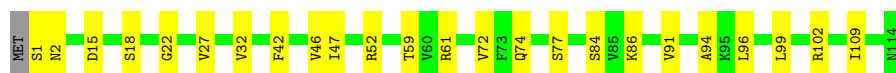
- Molecule 39: 50S ribosomal protein L18

Chain o: 75% 22% ..




- Molecule 40: 50S ribosomal protein L19

Chain p: 78% 21% .




- Molecule 41: 50S ribosomal protein L20

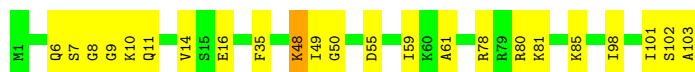


Chain q:  79% 18% ..




- Molecule 42: 50S ribosomal protein L21

Chain r:  78% 21% .



- Molecule 43: 50S ribosomal protein L22

Chain s:  79% 21%




- Molecule 44: 50S ribosomal protein L23

Chain t:  73% 20% 7%



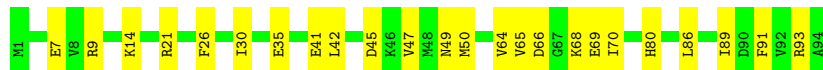
- Molecule 45: 50S ribosomal protein L24

Chain u:  86% 12% ..



- Molecule 46: 50S ribosomal protein L25

Chain v:  74% 26%




- Molecule 47: 50S ribosomal protein L27

Chain w:  69% 18% . 12%




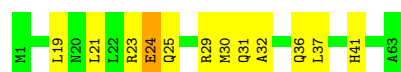
- Molecule 48: 50S ribosomal protein L28

Chain x:  79% 17% ..




- Molecule 49: 50S ribosomal protein L29

Chain y:  81% 17% .



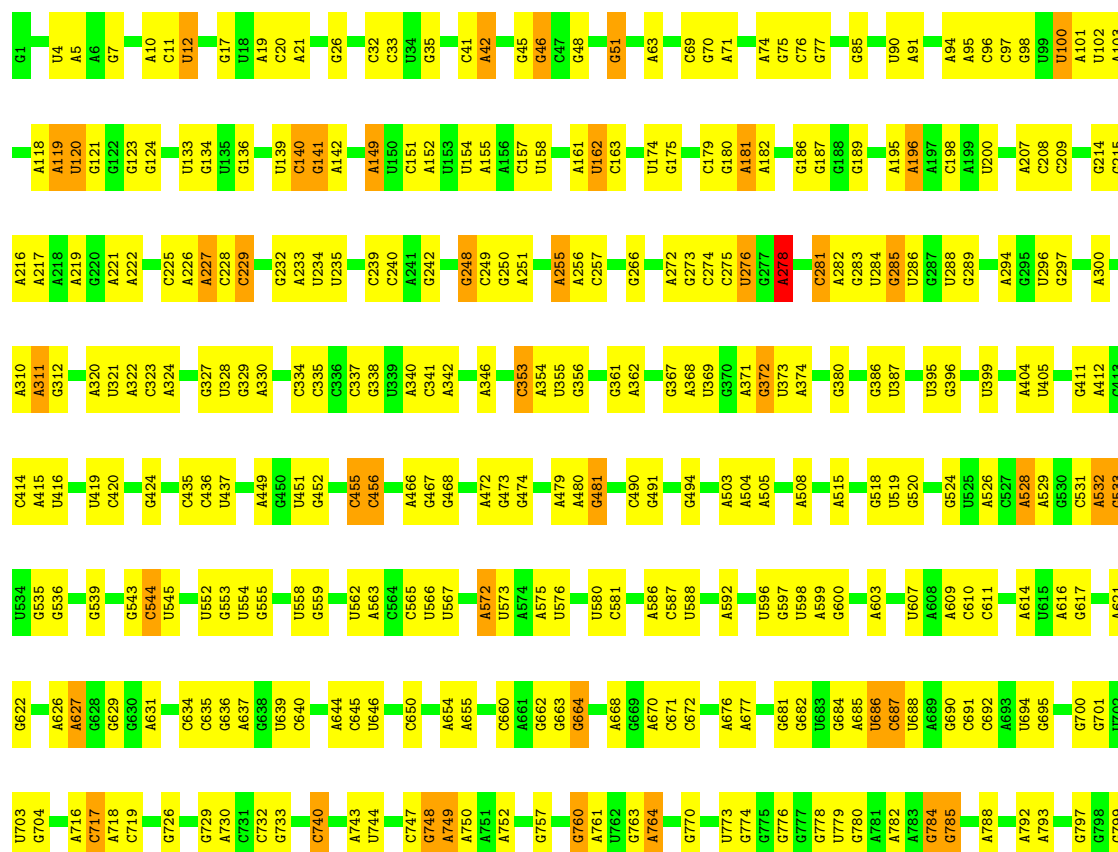
- Molecule 50: 50S ribosomal protein L30

Chain z:  78% 19% ..

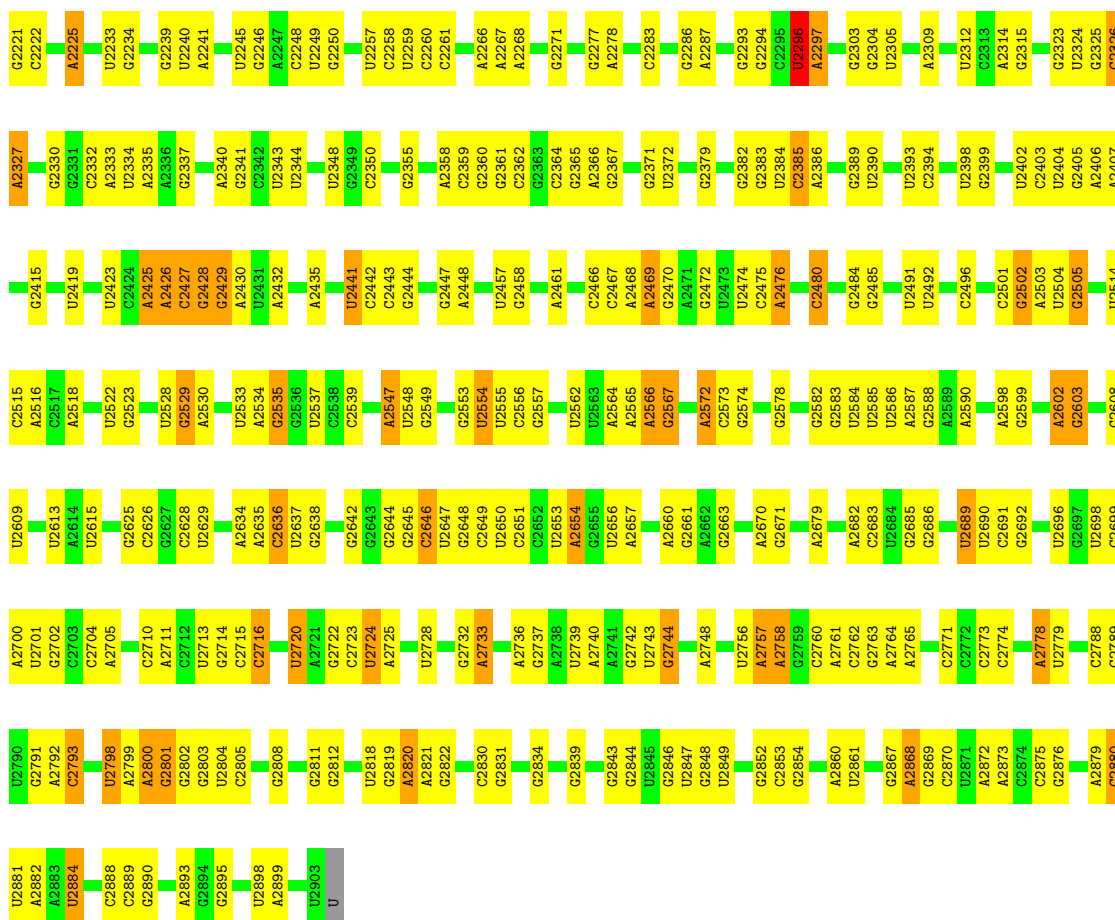


- Molecule 51: 23S rRNA

Chain 1:  56% 38% 6%

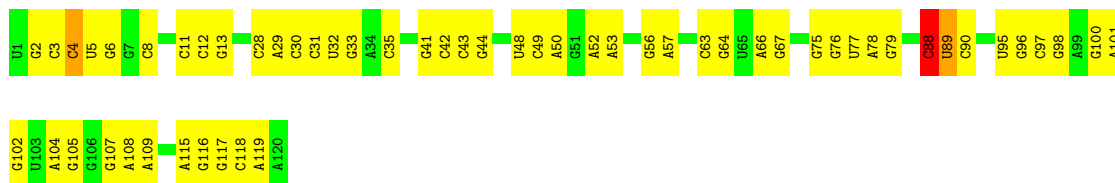


C2146	C2147	U2068	A1970	A1877	U1782	G1674	G1560	U1468	G1364	G1256	U1130	U1061	A983	U887	A800
A2071	A2072	G2069	U1971	G1878	A1783	C1675	C1564	A1469	A1365	C1257	G1131	G1062	A984	G801	G800
C2072	C1974	A2071	G1972	U1882	A1785	A1676	C1565	G1470	U1375	U1258	A1133	C1063	C986	A892	A802
C2163	U1991	C2072	C1974	U1883	A1786	U1680	G1568	C1472	G1377	G1259	C1134	C1064	C987	U894	C893
A2077	C1893	A2077	U1991	C1893	C1790	G1682	A1569	U1474	A1378	U1263	G1136	U1066	C989	U895	G805
A2080	C1894	U2080	G1992	C1894	A1791	U1697	U1578	G1475	G1380	G1271	G1137	G1067	A990	A896	C806
U2081	A1899	U2081	U1993	A1899	C1794	A1698	U1584	G1478	U1386	A1272	G1138	A1069	C994	U807	U808
U2086	C1996	U2086	C1996	A1900	C1795	A1698	U1584	G1478	A1383	A1273	G1139	A1070	C995	U809	G809
G2087	A1901	G2087	A1998	A1901	U1796	G1702	G1587	G1482	C1386	A1274	G1140	G1071	A996	U810	U811
A2090	G1906	A2090	C1999	G1906	U1798	U1709	C1595	A1490	A1387	G1277	A1143	G1074	U999	G907	C812
C2091	C1907	C2091	G1907	C1907	G1799	G1710	A1596	G1491	U1394	C1278	A1155	C1075	A1000	C908	U813
U2092	C1908	U2092	C1908	A1809	A1807	G1718	A1603	G1492	U1394	G1279	A1156	C1076	A1001	A910	C814
G2093	C1914	G2093	A1915	U1915	A1809	U1725	A1608	C1493	U1397	A1287	G1157	U1077	C1006	A919	C815
A2094	U1916	A2094	A1916	U1916	A1810	C1726	A1611	A1494	C1398	G1288	G1158	C1079	C1006	G914	C816
A2095	U1917	A2095	U1917	U1917	A1811	G1727	C1611	A1495	U1409	C1289	U1159	A1080	G1011	C915	C817
A2097	A1918	A2097	A1918	U1918	C1816	G1728	A1616	A1504	G1410	C1289	U1160	A1081	G1011	G916	C818
G2100	G1922	G2100	G1922	U1922	A1819	U1729	A1618	A1505	G1416	G1290	G1161	U1082	U1012	A917	U827
C2104	C1923	C2104	C1923	U1923	A1820	G1730	A1618	A1506	G1417	A1301	C1161	U1083	C1013	A918	U828
U2106	C1924	U2106	C1924	U1924	A1821	G1731	C1618	A1507	G1418	G1300	G1162	U1084	C1014	A919	A829
G2107	C1925	G2107	C1925	U1925	A1822	G1732	C1618	A1508	G1419	A1301	G1163	A1085	U1015	A920	G830
A2108	U1926	A2108	U1926	U1926	C1823	G1733	C1618	A1509	G1420	G1309	G1164	U1086	U1016	U929	G831
C2115	A1927	C2115	A1927	U1927	A1824	G1734	C1618	A1510	G1421	G1310	G1165	U1087	U1017	U832	G832
G2116	C1928	G2116	C1928	U1928	A1825	G1735	C1618	A1511	G1422	G1311	G1166	U1088	U1018	U833	A833
A2117	U1931	A2117	U1931	U1931	A1826	G1736	C1618	A1512	G1423	G1312	G1167	U1089	U1019	U834	U834
U2118	A1932	U2118	A1932	U1932	A1827	G1737	C1618	A1513	G1424	G1313	G1168	U1090	U1020	C935	C840
G2119	C1933	G2119	C1933	U1933	A1828	G1738	C1618	A1514	G1425	G1314	G1169	U1091	U1021	C936	A845
A2121	U1934	A2121	U1934	U1934	A1829	G1739	C1618	A1515	G1426	G1315	G1170	U1092	U1022	A937	U846
U2122	C1935	U2122	C1935	U1935	A1830	G1740	C1618	A1516	G1427	G1316	G1171	U1093	U1023	C938	G855
G2123	A1936	G2123	A1936	U1936	A1831	G1741	C1618	A1517	G1428	G1317	G1172	U1094	U1024	C939	G856
C2124	U1937	C2124	U1937	U1937	A1832	G1742	C1618	A1518	G1429	G1318	G1173	U1095	U1025	C940	G857
U2125	A1938	U2125	A1938	U1938	A1833	G1743	C1618	A1519	G1430	G1319	G1174	U1096	U1026	C941	G858
A2126	C1939	A2126	C1939	U1939	A1834	G1744	C1618	A1520	G1431	G1320	G1175	U1097	U1027	C942	G859
G2127	U1940	G2127	U1940	U1940	A1835	G1745	C1618	A1521	G1432	G1321	G1176	U1098	U1028	C943	G860
C2128	A1941	C2128	A1941	U1941	A1836	G1746	C1618	A1522	G1433	G1322	G1177	U1099	U1029	C944	U861
U2132	U1942	U2132	U1942	U1942	A1837	G1747	C1618	A1523	G1434	G1323	G1178	U1100	U1030	C945	U862
G2133	C1943	G2133	C1943	U1943	A1838	G1748	C1618	A1524	G1435	G1324	G1179	U1101	U1031	C946	A863
A2134	U1944	A2134	U1944	U1944	A1839	G1749	C1618	A1525	G1436	G1325	G1180	U1102	U1032	C947	G864
U2138	C1945	U2138	C1945	U1945	A1840	G1750	C1618	A1526	G1437	G1326	G1181	U1103	U1033	C948	G865
G2139	U1946	G2139	U1946	U1946	A1841	G1751	C1618	A1527	G1438	G1327	G1182	U1104	U1034	C949	U866
C2140	A1947	C2140	A1947	U1947	A1842	G1752	C1618	A1528	G1439	G1328	G1183	U1105	U1035	C950	G867
G2141	U1948	G2141	U1948	U1948	A1843	G1753	C1618	A1529	G1440	G1329	G1184	U1106	U1036	C951	U868
C2145	C1949	C2145	C1949	U1949	A1844	G1754	C1618	A1530	G1441	G1330	G1185	U1107	U1037	C952	U869
U2220	A1950	U2220	A1950	U1950	A1845	G1755	C1618	A1531	G1442	G1331	G1186	U1108	U1038	C953	U870
C2146	U1951	C2146	U1951	U1951	A1846	G1756	C1618	A1532	G1443	G1332	G1187	U1109	U1039	C954	U871
U2221	C1952	U2221	C1952	U1952	A1847	G1757	C1618	A1533	G1444	G1333	G1188	U1110	U1040	C955	U872
C2147	U1953	C2147	U1953	U1953	A1848	G1758	C1618	A1534	G1445	G1334	G1189	U1111	U1041	C956	U873
U2222	A1954	U2222	A1954	U1954	A1849	G1759	C1618	A1535	G1446	G1335	G1190	U1112	U1042	C957	C876
C2148	U1955	C2148	U1955	U1955	A1850	G1760	C1618	A1536	G1447	G1336	G1191	U1113	U1043	C958	C877
U2223	C1956	U2223	C1956	U1956	A1851	G1761	C1618	A1537	G1448	G1337	G1192	U1114	U1044	C959	C878
G2204	U1957	G2204	U1957	U1957	A1852	G1762	C1618	A1538	G1449	G1338	G1193	U1115	U1045	C960	U879
A2205	A1958	A2205	A1958	U1958	A1853	G1763	C1618	A1539	G1450	G1339	G1194	U1116	U1046	C961	A877
C2206	U1959	C2206	U1959	U1959	A1854	G1764	C1618	A1540	G1451	G1340	G1195	U1117	U1047	C962	A878
U2207	C1960	U2207	C1960	U1960	A1855	G1765	C1618	A1541	G1452	G1341	G1196	U1118	U1048	C963	C879
C2208	U1961	C2208	U1961	U1961	A1856	G1766	C1618	A1542	G1453	G1342	G1197	U1119	U1049	C964	C880
U2209	A1962	U2209	A1962	U1962	A1857	G1767	C1618	A1543	G1454	G1343	G1198	U1120	U1050	C965	U870
A2210	U1963	A2210	U1963	U1963	A1858	G1768	C1618	A1544	G1455	G1344	G1199	U1121	U1051	C966	U871
C2211	C1964	C2211	C1964	U1964	A1859	G1769	C1618	A1545	G1456	G1345	G1200	U1122	U1052	C967	U872
U2212	U1965	U2212	U1965	U1965	A1860	G1770	C1618	A1546	G1457	G1346	G1201	U1123	U1053	C968	C873
C2215	A1966	C2215	A1966	U1966	A1861	G1771	C1618	A1547	G1458	G1347	G1202	U1124	U1054	C969	U873
G2216	U1967	G2216	U1967	U1967	A1862	G1772	C1618	A1548	G1459	G1348	G1203	U1125	U1055	C970	U874
U2220	C1968	U2220	C1968	U1968	A1863	G1773	C1618	A1549	G1460	G1349	G1204	U1126	U1056	C971	U875
C2149	U1969	C2149	U1969	U1969	A1864	G1774	C1618	A1550	G1461	G1350	G1205	U1127	U1057	C972	A876
U2221	A1970	U2221	A1970	U1970	A1865	G1775	C1618	A1551	G1462	G1351	G1206	U1128	U1058	C973	A877
C2150	U1971	C2150	U1971	U1971	A1866	G1776	C1618	A1552	G1463	G1352	G1207	U1129	U1059	C974	A878
U2222	C1972	U2222	C1972	U1972	A1867	G1777	C1618	A1553	G1464	G1353	G1208	U1130	U1060	C975	A879
C2151	U1973	C2151	U1973	U1973	A1868	G1778	C1618	A1554	G1465	G1354	G1209	U1131	U1061	C976	C880
U2223	A1974	U2223	A1974	U1974	A1869	G1779	C1618	A1555	G1466	G1355	G1210	U1132	U1062	C977	U880
C2152	U1975	C2152	U1975	U1975	A1870	G1780	C1618	A1556	G1467	G1356	G1211	U1133	U1063	C978	U881
U2224	A1976	U2224	A1976	U1976	A1871	G1781	C1618	A1557	G1468	G1357	G1212	U1134	U1064	C979	U882
C2153	U1977	C2153	U1977	U1977	A1872	G1782	C1618	A1558	G1469	G1358	G1213	U1135	U1065	C980	U883
U2225	C1978	U2225	C1978	U1978	A1873	G1783	C1618	A1559	G1470	G1359	G1214	U1136	U1066	C981	U884
C2154	U1979	C2154	U1979	U1979	A1874	G1784	C1618	A1560	G1471	G1360	G1215	U1137	U1067	C982	U885
U2226	A1980	U2226	A1980	U1980	A1875	G1785	C1618	A1561	G1472	G1361	G1216	U1138	U1068	C983	U886
C2155	U1981	C2155	U1981	U1981	A1876	G1786	C1618	A1562	G1473	G1362	G1217	U1139	U1069	C984	U887
U2227	C1982	U2227	C1982	U1982	A1877	G1787	C1618	A1563	G1474	G1363	G1218	U1140	U1070	C985	U888
C2156	U1983	C2156	U1983	U1983	A1878	G1788	C1618	A1564	G1475	G1364	G1219	U1141	U1071	C986	U889
U2228	A1984	U2228	A1984	U1984	A1879	G1789	C1618	A1565	G1476	G1365	G1220	U1142	U1072	C987	U890
C2157	U1985	C2157	U1985	U1985	A1880	G1790	C1618	A1566	G1477	G1366	G1221	U1143	U1073	C988	U891
U2229	C1986	U2229	C1986	U1986	A1881	G1791	C1618	A1567	G1478	G1367	G1222	U1144	U1074	C989	U892
C2158	U1987	C2158	U1987	U1987	A1882	G1792	C1618	A1568	G1479	G1368	G1223	U1145	U1075	C990	U893
U2230	A1988	U2230	A1988	U1988	A1883	G1793	C1618	A1569	G1480	G1369	G1224	U1146	U1076	C991	U894
C2159	U1989	C2159	U1989</												



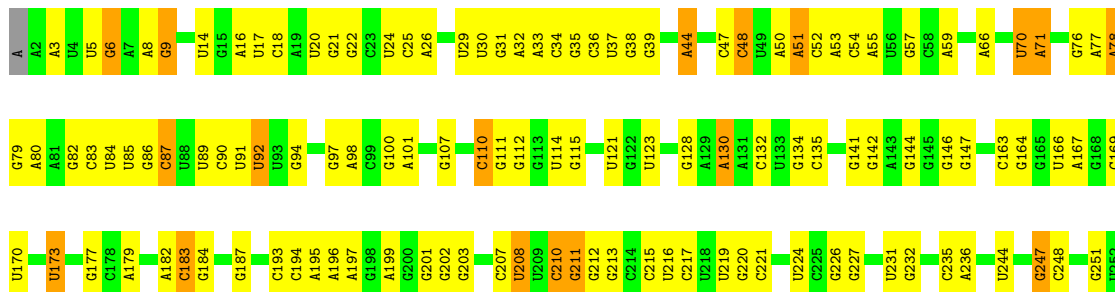
• Molecule 52: 5S rRNA

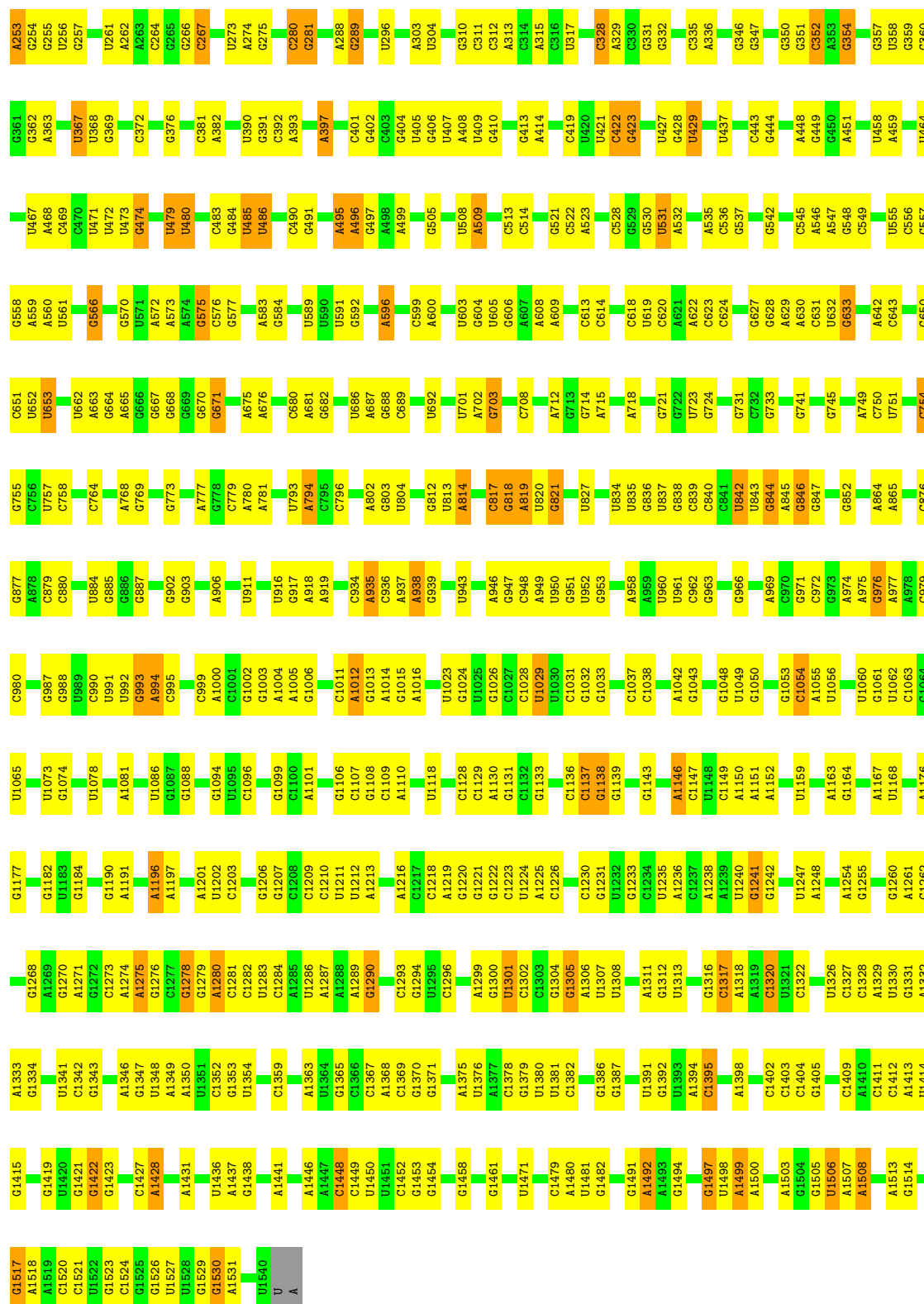
Chain 2: 53% 44%



• Molecule 53: 16S rRNA

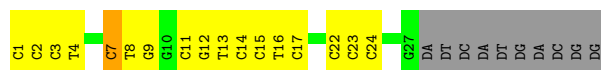
Chain 3: 55% 39% 6%



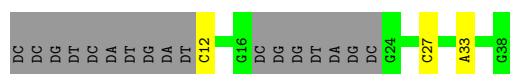




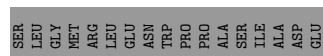
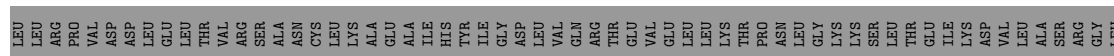
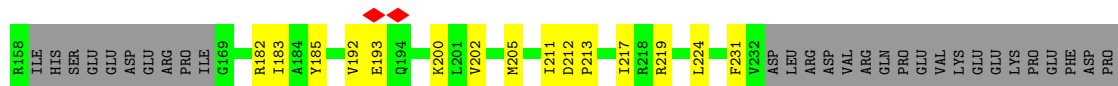
- Molecule 55: template DNA strand



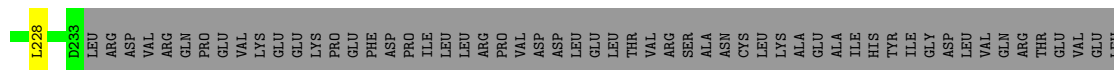
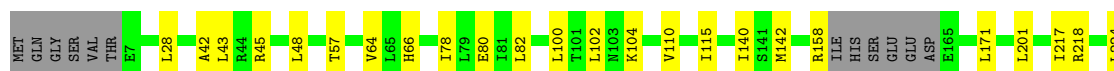
- Molecule 56: non-template DNA strand



- Molecule 57: DNA-directed RNA polymerase subunit alpha

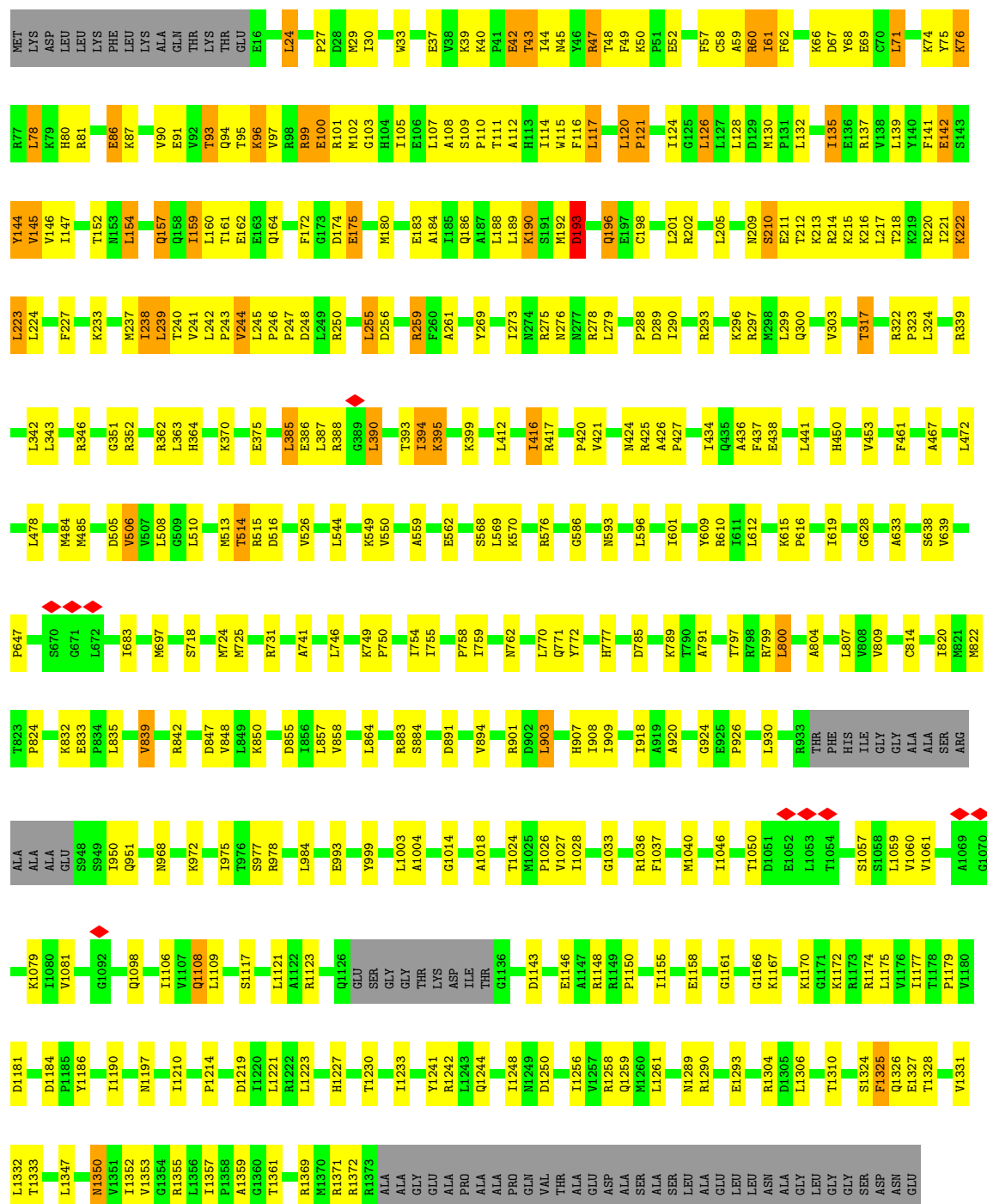


- Molecule 57: DNA-directed RNA polymerase subunit alpha



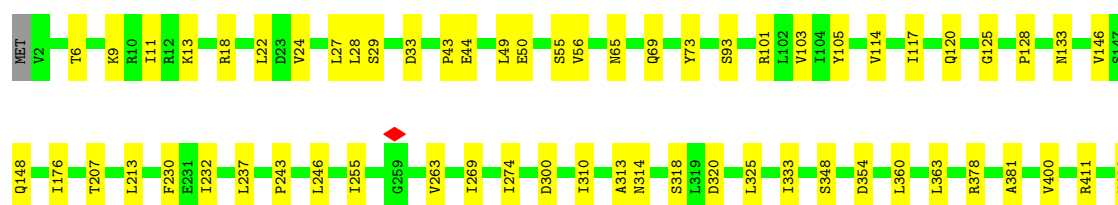
- Molecule 58: DNA-directed RNA polymerase subunit beta'

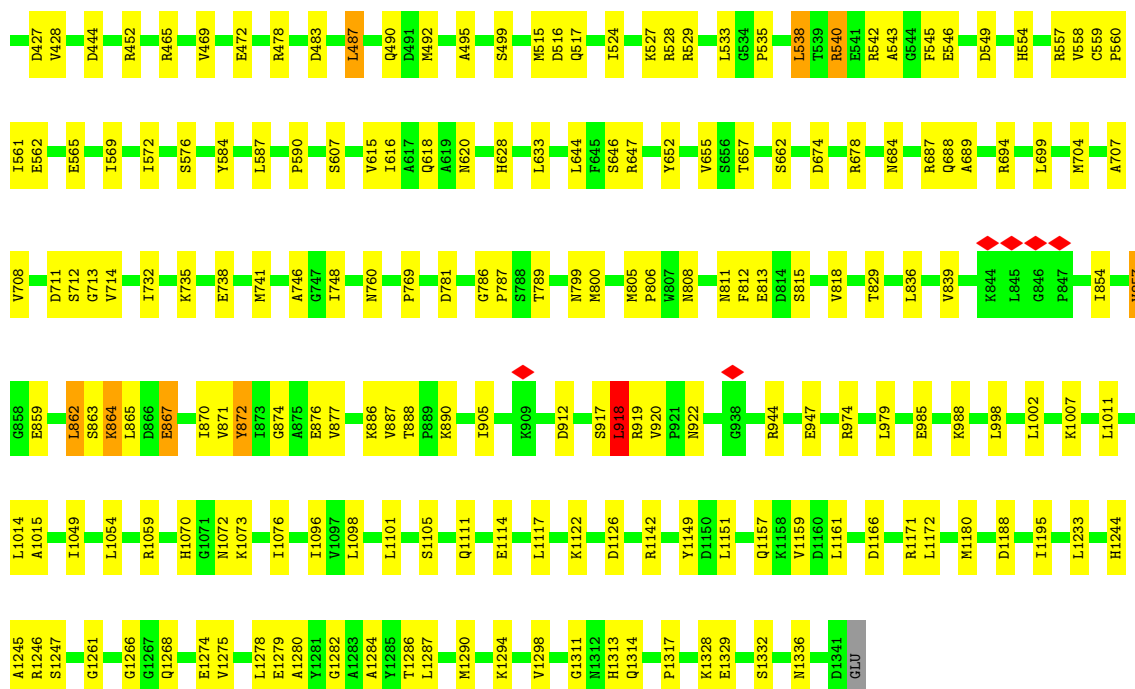




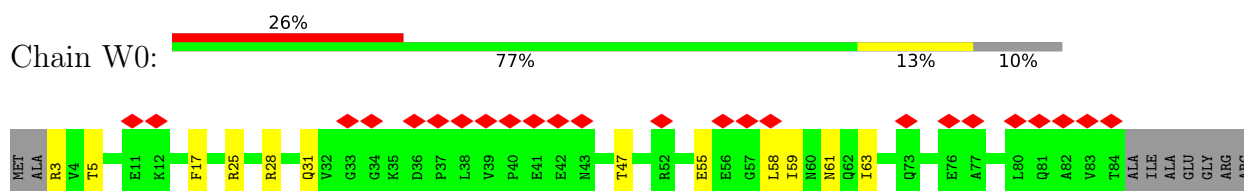
• Molecule 59: DNA-directed RNA polymerase subunit beta

Chain B2: 81% 18%.

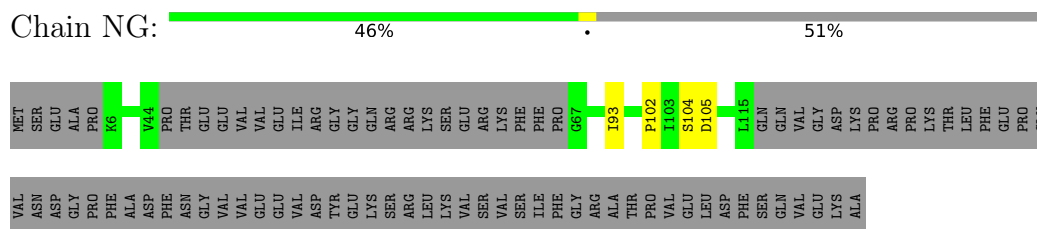




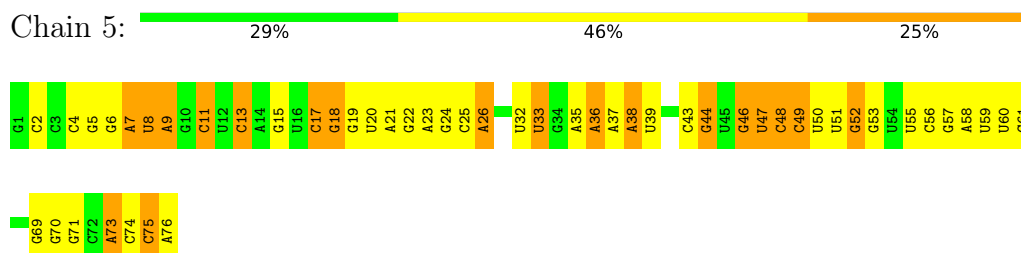
- Molecule 60: DNA-directed RNA polymerase subunit omega



- Molecule 61: Transcription termination/antitermination protein NusG



- Molecule 62: tRNA(Phe)



- Molecule 63: tRNA(fMet)

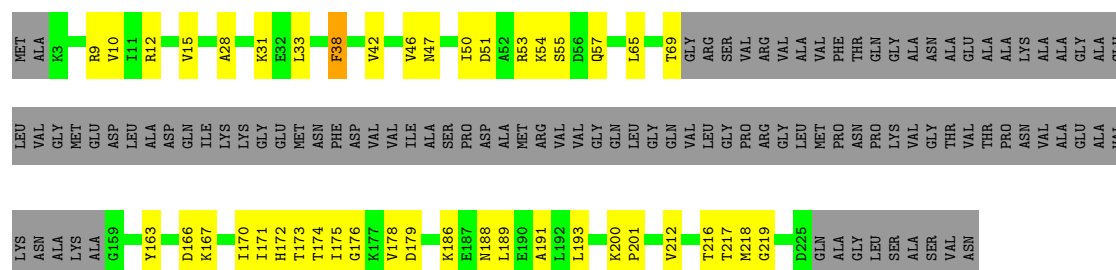


Chain 6:  58% 30% 12%



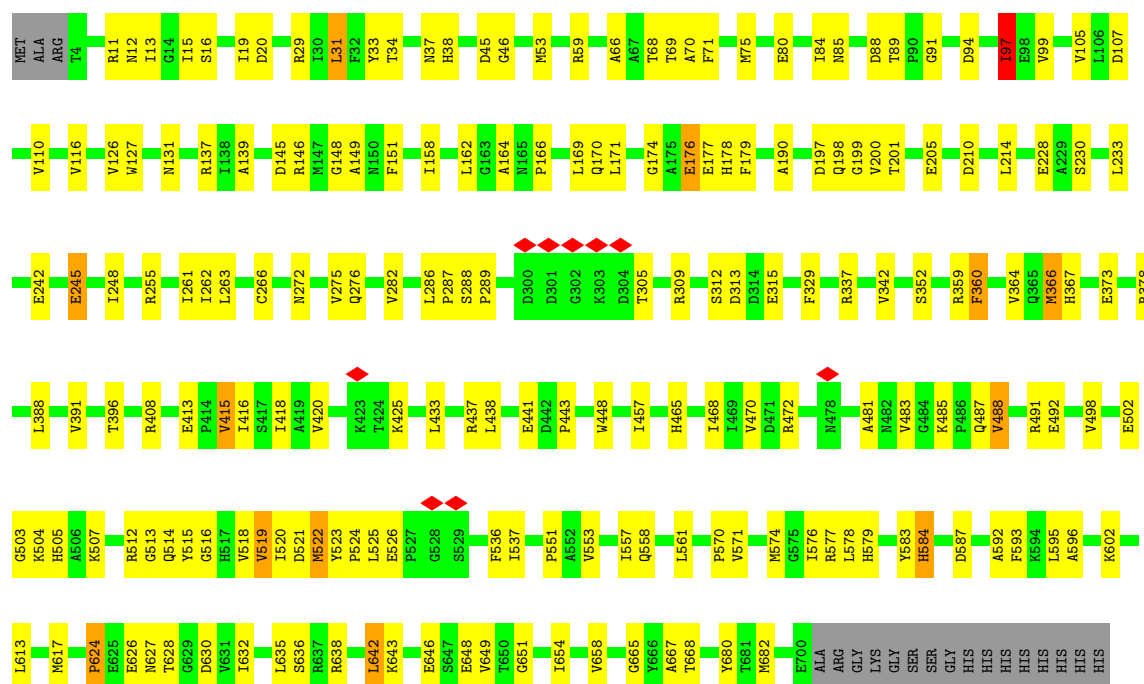
• Molecule 64: Large ribosomal subunit protein uL1

Chain a:  39% 18% 43%



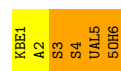
• Molecule 65: Elongation factor G

Chain 0:  70% 26% • •



• Molecule 66: Viomycin

Chain h:  33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	626298	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size ( $\text{\AA}$ )	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.57, 1.57, 1.57	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5OH, UAL, PO4, DPP, KBE, MG, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/531	0.99	4/709 (0.6%)
2	B	0.51	0/450	0.84	0/599
3	C	0.35	0/416	0.73	0/554
4	D	0.41	0/380	0.89	1/498 (0.2%)
5	E	0.49	0/513	0.87	0/676
6	F	0.34	0/303	0.77	0/397
7	G	0.48	0/1735	0.93	8/2338 (0.3%)
8	H	0.51	0/1647	0.94	4/2221 (0.2%)
9	I	0.46	0/1665	0.98	7/2227 (0.3%)
10	J	0.53	0/1165	0.94	5/1568 (0.3%)
11	K	0.58	0/835	1.02	5/1128 (0.4%)
12	L	0.45	0/1195	1.02	8/1602 (0.5%)
13	M	0.38	0/989	0.80	0/1326
14	N	0.55	0/1034	1.09	6/1375 (0.4%)
15	O	0.58	0/796	1.05	3/1077 (0.3%)
16	P	0.41	0/885	0.98	6/1195 (0.5%)
17	Q	0.62	1/969 (0.1%)	1.05	5/1300 (0.4%)
18	R	0.39	0/892	0.87	1/1193 (0.1%)
19	S	0.39	0/817	0.90	2/1088 (0.2%)
20	T	0.41	0/722	0.84	0/964
21	U	0.40	0/659	0.91	2/884 (0.2%)
22	V	0.41	0/657	0.85	2/881 (0.2%)
23	W	0.47	0/544	0.95	2/731 (0.3%)
24	X	0.40	0/652	0.95	1/877 (0.1%)
25	Y	0.38	0/671	0.90	2/888 (0.2%)
26	Z	0.60	0/550	1.12	2/728 (0.3%)
27	b	0.45	0/2121	0.93	6/2852 (0.2%)
28	c	0.39	0/1586	0.84	4/2134 (0.2%)
29	d	0.43	0/1571	0.78	0/2113
30	e	0.43	0/1434	0.87	3/1926 (0.2%)
31	f	0.41	0/1343	0.82	2/1816 (0.1%)
32	g	0.47	0/1122	0.93	3/1515 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	i	0.70	1/1046 (0.1%)	1.16	6/1410 (0.4%)
34	j	0.39	0/1152	0.86	4/1551 (0.3%)
35	k	0.50	0/947	0.92	1/1268 (0.1%)
36	l	0.41	0/1054	0.95	4/1403 (0.3%)
37	m	0.39	0/1093	0.85	3/1460 (0.2%)
38	n	0.39	0/973	0.92	3/1301 (0.2%)
39	o	0.39	0/902	0.92	3/1209 (0.2%)
40	p	0.40	0/929	0.85	1/1242 (0.1%)
41	q	0.48	0/960	0.86	1/1278 (0.1%)
42	r	0.49	0/829	0.96	1/1107 (0.1%)
43	s	0.39	0/864	0.84	2/1156 (0.2%)
44	t	0.39	0/744	0.78	0/994
45	u	0.41	0/784	0.92	3/1047 (0.3%)
46	v	0.39	0/766	0.78	0/1025
47	w	0.34	0/582	0.72	0/769
48	x	0.37	0/635	0.85	2/848 (0.2%)
49	y	0.34	0/510	0.87	1/677 (0.1%)
50	z	0.50	0/453	0.75	0/605
51	1	0.44	0/69796	0.54	8/108888 (0.0%)
52	2	0.45	0/2872	0.53	1/4479 (0.0%)
53	3	0.45	0/36963	0.53	3/57662 (0.0%)
54	4	0.56	0/431	0.62	0/668
55	8	0.56	0/599	0.71	1/919 (0.1%)
56	9	0.48	0/468	0.52	0/719
57	A1	0.48	0/1696	0.69	0/2298
57	A2	0.42	0/1718	0.62	0/2328
58	B1	0.56	4/10510 (0.0%)	0.74	8/14196 (0.1%)
59	B2	0.47	0/10663	0.68	2/14396 (0.0%)
60	W0	0.29	0/652	0.61	0/879
61	NG	0.55	0/431	0.79	0/596
62	5	0.56	0/1812	0.88	2/2823 (0.1%)
63	6	0.43	0/1832	0.56	0/2855
64	a	0.47	0/1033	0.98	5/1387 (0.4%)
65	0	0.51	0/5501	0.96	19/7446 (0.3%)
66	h	3.19	2/11 (18.2%)	0.75	0/13
All	All	0.46	8/193060 (0.0%)	0.68	178/284282 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	h	3	SER	CA-C	-6.76	1.38	1.52
66	h	4	SER	CA-C	-6.20	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.25	1.22	1.33
33	i	2	LYS	N-CA	5.17	1.49	1.46
58	B1	424	ASN	CG-ND2	-5.14	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.07	1.33	1.23
58	B1	777	HIS	ND1-CE1	5.06	1.37	1.32
17	Q	43	LYS	N-CA	5.05	1.50	1.46

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	57	VAL	N-CA-C	-10.06	103.67	112.12
65	0	174	GLY	N-CA-C	10.05	123.42	111.35
11	K	99	ALA	N-CA-C	9.92	123.42	111.02
64	a	179	ASP	N-CA-C	-9.71	99.89	114.64
16	P	73	VAL	N-CA-C	-9.11	104.45	113.20
8	H	124	GLU	N-CA-C	-8.92	101.47	111.82
65	0	45	ASP	N-CA-C	-8.85	103.60	114.75
8	H	9	ILE	N-CA-C	8.73	115.55	106.21
12	L	111	GLY	N-CA-C	8.60	121.42	111.36
15	O	60	ASP	N-CA-C	-8.58	104.83	114.62
9	I	7	LYS	N-CA-C	8.45	121.71	111.40
39	o	22	GLY	N-CA-C	-8.44	101.22	111.35
43	s	24	ILE	N-CA-C	8.42	115.22	106.21
37	m	60	GLN	N-CA-C	8.26	122.40	110.10
1	A	45	THR	N-CA-C	-8.23	102.69	112.89
15	O	91	ASP	N-CA-C	-8.10	104.27	114.56
51	1	876	C	C2'-C3'-O3'	-8.10	101.56	113.70
65	0	38	HIS	N-CA-C	-7.85	97.61	109.94
65	0	413	GLU	N-CA-C	7.73	119.52	109.93
33	i	90	GLY	N-CA-C	-7.70	105.31	114.48
7	G	88	GLN	N-CA-C	7.66	121.73	110.17
31	f	46	ASP	N-CA-C	-7.52	103.02	111.14
51	1	1020	A	C2'-C3'-O3'	7.36	120.53	109.50
9	I	168	THR	N-CA-C	7.26	122.19	111.96
34	j	105	VAL	N-CA-C	-7.13	106.12	111.90
64	a	10	VAL	N-CA-C	-7.06	103.59	110.72
4	D	7	PRO	N-CA-C	7.04	122.40	111.21
27	b	87	SER	N-CA-C	-7.01	105.26	113.88
10	J	73	VAL	N-CA-C	-7.00	106.67	113.53
16	P	126	ARG	N-CA-C	6.95	119.04	110.91
19	S	39	ASP	N-CA-C	-6.91	103.85	112.90
26	Z	66	ARG	N-CA-C	6.87	119.61	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	91	ARG	CA-C-N	6.83	126.07	118.97
12	L	91	ARG	C-N-CA	6.83	126.07	118.97
33	i	119	ALA	N-CA-C	6.80	120.34	110.42
1	A	54	GLY	N-CA-C	6.79	123.30	112.58
39	o	10	ARG	N-CA-C	-6.78	105.16	113.50
65	0	366	MET	N-CA-C	6.78	118.84	110.91
64	a	178	VAL	N-CA-C	6.74	113.42	106.21
21	U	46	LYS	N-CA-C	-6.63	99.02	109.50
34	j	81	ILE	N-CA-C	6.62	117.31	110.36
48	x	17	ARG	N-CA-C	6.58	119.24	111.02
58	B1	450	HIS	CB-CG-CD2	-6.55	122.69	131.20
27	b	30	ALA	N-CA-C	6.51	121.60	112.75
27	b	121	ALA	N-CA-C	6.50	118.68	110.24
21	U	79	ASN	N-CA-C	6.49	118.70	110.33
27	b	248	GLY	N-CA-C	6.46	122.92	113.48
24	X	48	ILE	N-CA-C	6.44	118.06	109.37
28	c	59	ARG	N-CA-C	-6.43	107.29	114.62
30	e	43	ILE	N-CA-C	-6.36	103.15	111.09
30	e	147	ARG	N-CA-C	6.33	118.04	110.19
58	B1	777	HIS	CB-CG-CD2	-6.32	122.98	131.20
58	B1	61	ILE	CA-C-N	-6.31	114.07	121.64
58	B1	61	ILE	C-N-CA	-6.31	114.07	121.64
38	n	104	ALA	N-CA-C	6.27	118.92	111.71
25	Y	6	ALA	N-CA-C	-6.22	103.37	113.19
16	P	90	PRO	N-CA-C	-6.21	105.54	114.18
33	i	21	PRO	N-CA-C	6.20	118.26	110.70
36	l	95	LEU	N-CA-C	-6.17	105.58	113.23
12	L	86	VAL	N-CA-C	6.14	114.73	109.02
16	P	125	LYS	N-CA-C	6.14	123.89	110.80
45	u	6	ARG	N-CA-C	6.13	123.85	110.80
10	J	11	GLN	N-CA-C	6.12	119.68	111.24
23	W	68	PRO	N-CA-C	6.10	120.55	111.41
9	I	177	MET	N-CA-C	6.05	117.99	110.91
18	R	14	ALA	N-CA-C	6.05	118.67	111.71
12	L	135	LYS	N-CA-C	-6.04	105.95	113.38
38	n	14	SER	N-CA-C	6.04	117.54	111.07
65	0	408	ARG	N-CA-C	6.04	118.58	108.73
10	J	110	MET	N-CA-C	-6.02	105.85	113.43
7	G	212	TYR	N-CA-C	6.01	117.70	111.03
34	j	31	GLU	N-CA-C	-6.01	104.85	111.82
11	K	86	ARG	N-CA-C	6.01	117.94	110.91
37	m	110	GLU	N-CA-C	6.00	117.49	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	43	LYS	N-CA-C	5.98	117.60	111.14
14	N	58	GLU	N-CA-C	-5.93	104.91	113.21
48	x	60	LYS	N-CA-C	-5.92	104.46	111.03
1	A	43	PHE	N-CA-C	-5.92	106.19	113.41
27	b	145	MET	N-CA-C	-5.91	106.71	114.04
14	N	42	THR	N-CA-C	5.89	119.77	111.52
36	l	115	GLU	N-CA-C	5.88	117.80	110.91
30	e	4	HIS	N-CA-C	-5.85	104.49	111.69
7	G	13	VAL	N-CA-C	5.84	121.48	109.34
51	1	1085	A	C2'-C3'-O3'	-5.81	104.98	113.70
52	2	88	C	C2'-C3'-O3'	-5.80	104.99	113.70
8	H	10	ARG	N-CA-C	-5.80	105.57	114.16
8	H	5	HIS	N-CA-C	5.77	116.67	109.57
12	L	90	VAL	N-CA-C	5.77	117.64	108.87
17	Q	33	CYS	N-CA-C	5.77	117.66	110.91
45	u	89	GLY	N-CA-C	-5.76	107.19	114.16
28	c	86	GLU	N-CA-C	5.76	119.19	111.24
7	G	123	GLY	N-CA-C	5.70	117.31	111.56
58	B1	450	HIS	CB-CG-ND1	5.67	131.21	122.70
41	q	75	TYR	N-CA-C	5.67	117.13	111.07
34	j	119	PHE	N-CA-C	-5.66	106.50	113.41
16	P	89	GLY	N-CA-C	5.65	123.87	112.34
33	i	53	PRO	N-CA-C	5.64	119.94	111.14
42	r	50	GLY	N-CA-C	-5.63	105.56	112.77
65	0	635	LEU	N-CA-C	-5.63	104.83	110.97
65	0	359	ARG	N-CA-C	5.62	117.15	110.19
14	N	71	ILE	N-CA-C	5.61	116.06	110.23
22	V	58	VAL	N-CA-C	5.60	116.65	107.24
33	i	124	MET	N-CA-C	-5.60	104.80	111.69
51	1	2296	U	C2'-C3'-O3'	-5.60	105.31	113.70
43	s	62	ASP	N-CA-C	5.59	118.45	111.24
39	o	21	LEU	N-CA-C	-5.58	105.08	113.89
35	k	108	ARG	N-CA-C	5.56	118.70	108.58
17	Q	117	GLY	N-CA-C	5.55	122.48	114.10
17	Q	115	LYS	N-CA-C	-5.53	101.52	110.32
45	u	31	GLY	N-CA-C	-5.51	107.17	114.95
65	0	31	LEU	N-CA-C	-5.51	105.68	112.90
62	5	73	A	C3'-C2'-O2'	5.51	118.96	110.70
11	K	39	LEU	N-CA-C	-5.51	104.42	113.50
7	G	151	LYS	N-CA-C	5.48	117.69	111.11
11	K	62	MET	N-CA-C	5.48	119.64	112.13
65	0	242	GLU	N-CA-C	-5.47	100.19	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	34	ARG	N-CA-C	5.46	122.44	110.80
65	0	37	ASN	N-CA-C	5.46	118.31	109.40
17	Q	22	ALA	N-CA-C	-5.46	105.24	111.14
58	B1	777	HIS	CB-CG-ND1	5.46	130.89	122.70
55	8	7	DC	C2'-C3'-O3'	-5.45	103.32	111.50
51	1	278	A	N9-C1'-C2'	5.44	120.16	112.00
9	I	13	ARG	N-CA-C	-5.43	106.66	113.28
23	W	51	GLN	N-CA-C	-5.42	106.34	113.12
65	0	287	PRO	N-CA-C	5.41	119.69	111.19
7	G	46	VAL	N-CA-CB	5.40	113.90	110.50
62	5	75	C	C4'-C3'-O3'	5.38	117.46	109.40
28	c	174	SER	N-CA-C	5.37	117.19	110.91
11	K	64	VAL	N-CA-C	5.37	115.69	108.17
22	V	79	GLU	N-CA-C	5.37	117.19	110.91
65	0	245	GLU	N-CA-C	5.37	118.62	111.75
49	y	24	GLU	N-CA-C	5.35	122.20	110.80
12	L	6	ILE	N-CA-C	5.34	120.46	109.34
51	1	1104	C	C4'-C3'-O3'	5.34	121.01	113.00
9	I	150	LYS	N-CA-C	5.32	117.14	110.91
33	i	72	THR	N-CA-C	-5.30	98.10	109.81
53	3	754	C	N1-C1'-C2'	5.29	119.93	112.00
59	B2	867	GLU	CA-C-N	-5.28	112.89	122.50
59	B2	867	GLU	C-N-CA	-5.28	112.89	122.50
65	0	46	GLY	N-CA-C	-5.26	108.06	115.32
31	f	174	LYS	N-CA-C	5.25	121.99	110.80
9	I	182	LYS	N-CA-C	5.25	119.32	112.13
10	J	160	VAL	N-CA-C	5.23	115.95	110.62
12	L	129	ASN	N-CA-C	5.22	118.40	111.30
58	B1	27	PRO	N-CA-C	-5.22	106.24	113.81
65	0	97	ILE	N-CA-C	-5.22	105.45	110.72
65	0	80	GLU	N-CA-C	-5.21	102.90	110.08
14	N	40	ARG	N-CA-C	-5.20	106.03	114.09
65	0	441	GLU	N-CA-C	5.20	117.94	111.24
32	g	63	ALA	N-CA-C	-5.19	106.90	113.18
65	0	624	PRO	N-CA-C	5.17	120.33	113.40
19	S	13	VAL	N-CA-C	-5.16	105.38	111.00
64	a	38	PHE	N-CA-C	-5.14	100.79	109.07
32	g	136	SER	N-CA-C	5.13	121.74	110.80
38	n	50	PRO	N-CA-C	-5.12	107.45	113.86
51	1	100	U	N1-C1'-C2'	5.12	119.69	112.00
64	a	191	ALA	N-CA-C	-5.12	106.87	113.02
10	J	92	ARG	N-CA-CB	-5.12	104.48	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	56	LEU	N-CA-C	-5.12	105.78	111.36
15	O	38	GLY	N-CA-C	5.11	122.77	112.34
65	0	13	ILE	N-CA-C	5.11	116.65	108.89
14	N	103	VAL	N-CA-C	-5.10	107.84	112.12
36	l	29	LYS	CA-C-N	5.09	131.26	121.54
36	l	29	LYS	C-N-CA	5.09	131.26	121.54
58	B1	61	ILE	CA-C-O	-5.09	115.66	120.95
9	I	165	GLU	N-CA-C	5.09	121.64	110.80
53	3	1301	U	C4'-C3'-O3'	5.07	117.01	109.40
1	A	5	ILE	N-CA-C	-5.07	107.86	112.12
40	p	18	SER	N-CA-C	5.07	117.90	110.30
53	3	368	U	N1-C1'-C2'	5.07	119.60	112.00
27	b	157	ALA	N-CA-C	5.06	117.68	110.24
32	g	14	SER	N-CA-C	5.06	117.30	110.06
51	l	1111	A	N9-C1'-C2'	5.06	119.59	112.00
37	m	27	SER	N-CA-C	5.05	119.44	113.28
7	G	112	ARG	N-CA-C	-5.02	105.89	111.36
16	P	14	GLN	N-CA-C	5.01	117.57	110.10
28	c	143	PRO	N-CA-C	5.01	120.44	113.98
17	Q	54	VAL	N-CA-C	5.01	115.52	108.36

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	522	0	524	19	0
2	B	444	0	461	10	0
3	C	409	0	440	7	0
4	D	377	0	418	14	0
5	E	504	0	574	9	0
6	F	302	0	341	10	0
7	G	1704	0	1732	25	0
8	H	1620	0	1688	36	0
9	I	1643	0	1710	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1152	0	1195	21	0
11	K	817	0	808	16	0
12	L	1181	0	1240	27	0
13	M	979	0	1034	13	0
14	N	1022	0	1070	35	0
15	O	786	0	828	28	0
16	P	869	0	878	23	0
17	Q	955	0	1019	17	0
18	R	883	0	944	21	0
19	S	805	0	847	21	0
20	T	714	0	737	12	0
21	U	649	0	666	21	0
22	V	648	0	691	20	0
23	W	535	0	552	14	0
24	X	637	0	665	22	0
25	Y	665	0	714	21	0
26	Z	544	0	579	10	0
27	b	2082	0	2157	54	0
28	c	1565	0	1616	36	0
29	d	1552	0	1619	25	0
30	e	1410	0	1447	28	0
31	f	1323	0	1374	20	0
32	g	1111	0	1148	19	0
33	i	1032	0	1088	59	0
34	j	1129	0	1162	21	0
35	k	938	0	1012	19	0
36	l	1045	0	1117	30	0
37	m	1074	0	1157	17	0
38	n	960	0	1000	20	0
39	o	892	0	923	21	0
40	p	917	0	965	21	0
41	q	947	0	1022	18	0
42	r	816	0	839	16	0
43	s	857	0	922	15	0
44	t	738	0	807	12	0
45	u	776	0	825	6	0
46	v	753	0	780	17	0
47	w	575	0	592	16	0
48	x	625	0	655	14	0
49	y	509	0	543	8	0
50	z	449	0	491	9	0
51	1	62317	0	31346	959	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	2	2568	0	1303	57	0
53	3	33012	0	16618	566	0
54	4	387	0	192	6	0
55	8	539	0	305	29	0
56	9	417	0	224	6	0
57	A1	1677	0	1713	27	0
57	A2	1698	0	1718	16	0
58	B1	10353	0	10548	330	0
59	B2	10496	0	10451	173	0
60	W0	650	0	658	10	0
61	NG	433	0	193	8	0
62	5	1622	0	821	23	0
63	6	1640	0	837	19	0
64	a	1026	0	1092	31	0
65	0	5399	0	5363	109	0
66	h	48	0	40	7	0
67	B1	1	0	0	0	0
68	0	28	0	12	2	0
69	0	5	0	0	1	0
All	All	179757	0	131050	2851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:42:ARG:NH2	53:3:721:G:H5''	1.59	1.17
35:k:48:PRO:HB3	53:3:1423:G:H5''	1.23	1.16
33:i:93:ASN:HB2	51:1:1077:A:H5'	1.12	1.07
51:1:2682:A:H61	51:1:2728:U:H1'	1.17	1.07
51:1:1064:C:H3'	51:1:1065:U:H5''	1.37	1.07
23:W:42:ARG:HH21	53:3:721:G:H5''	0.97	1.06
51:1:1019:U:OP1	51:1:1036:G:H5'	1.54	1.05
63:6:26:G:H2'	63:6:27:U:H5''	1.39	1.04
22:V:5:ARG:HH22	53:3:128:G:H5'	1.20	1.03
51:1:814:C:H1'	51:1:1225:G:H21	1.20	1.02
58:B1:750:PRO:HB3	59:B2:549:ASP:OD2	1.60	1.01
33:i:7:TYR:HE2	33:i:57:VAL:HB	1.24	1.01
51:1:1645:G:H5''	51:1:1646:C:H5'	1.42	1.01
58:B1:111:THR:HG23	58:B1:300:GLN:CD	1.86	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:41:PRO:HB3	53:3:1151:A:H1'	1.41	1.00
33:i:123:ALA:HB1	51:1:1081:U:H4'	1.44	1.00
33:i:92:PRO:HB2	51:1:1077:A:O4'	1.62	1.00
51:1:1557:C:H3'	51:1:1558:C:H5''	1.42	0.99
53:3:1421:G:H3'	53:3:1422:G:H4'	1.44	0.99
33:i:93:ASN:HB2	51:1:1077:A:C5'	1.93	0.98
1:A:64:PHE:HD1	53:3:1011:C:H4'	1.26	0.98
34:j:27:ARG:HH22	51:1:1142:A:H4'	1.29	0.97
58:B1:352:ARG:HD2	59:B2:1268:GLN:NE2	1.79	0.97
51:1:2382:G:H5''	51:1:2383:G:H5'	1.44	0.96
6:F:3:VAL:HG21	51:1:2539:C:H5'	1.47	0.95
22:V:5:ARG:NH2	53:3:128:G:H5'	1.83	0.94
51:1:1394:U:H4'	51:1:1603:A:H4'	1.49	0.94
58:B1:68:TYR:O	58:B1:75:TYR:CE2	2.20	0.94
65:0:524:PRO:HA	65:0:574:MET:HA	1.47	0.94
51:1:562:U:H2'	51:1:572:A:H1'	1.50	0.94
51:1:1098:A:H2'	51:1:1099:G:H5'	1.48	0.93
56:9:33:DA:H5''	58:B1:121:PRO:HG3	1.49	0.92
51:1:663:G:H2'	51:1:664:G:H5''	1.51	0.90
58:B1:202:ARG:HG2	58:B1:202:ARG:HH11	1.35	0.90
58:B1:68:TYR:C	58:B1:75:TYR:HE2	1.80	0.90
33:i:93:ASN:CB	51:1:1077:A:H5'	2.02	0.89
21:U:31:ARG:HB2	53:3:310:G:H5''	1.53	0.89
51:1:45:G:H5''	51:1:46:G:H5'	1.51	0.88
58:B1:317:THR:HA	58:B1:323:PRO:HA	1.55	0.88
51:1:1045:C:H5'	51:1:1046:A:C8	2.09	0.88
51:1:1697:G:H3'	51:1:1698:A:H5''	1.52	0.88
59:B2:854:ILE:HG21	59:B2:917:SER:HB3	1.54	0.87
62:5:9:A:H2'	62:5:11:C:H41	1.38	0.87
63:6:69:C:H2'	63:6:70:G:H5''	1.56	0.87
54:4:44:G:H21	58:B1:427:PRO:HD3	1.38	0.87
53:3:1421:G:N7	53:3:1422:G:H1'	1.89	0.87
55:8:1:DC:H5''	58:B1:210:SER:OG	1.75	0.86
58:B1:68:TYR:HB3	58:B1:75:TYR:OH	1.76	0.85
53:3:813:U:H2'	53:3:814:A:H5''	1.59	0.85
51:1:1075:C:H3'	51:1:1076:C:H5''	1.58	0.85
51:1:876:C:H3'	51:1:877:A:C4'	2.06	0.85
51:1:2653:U:H3'	51:1:2654:A:H5''	1.58	0.85
51:1:2656:U:H5''	65:0:146:ARG:HE	1.40	0.84
58:B1:68:TYR:O	58:B1:75:TYR:HE2	1.58	0.84
58:B1:633:ALA:HB2	59:B2:808:ASN:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:57:THR:HG21	53:3:362:G:H5''	1.57	0.83
21:U:14:ARG:HH12	53:3:618:C:H1'	1.43	0.83
2:B:5:ASN:HD22	51:1:2020:A:H62	1.24	0.83
15:O:43:PRO:HA	53:3:1151:A:H5'	1.59	0.83
21:U:5:ARG:HB2	53:3:376:G:H5''	1.59	0.83
46:v:49:ASN:HD21	51:1:1040:A:H4'	1.40	0.83
51:1:814:C:H1'	51:1:1225:G:N2	1.93	0.83
58:B1:289:ASP:HB2	61:NG:104:SER:CB	2.09	0.83
51:1:740:C:H6	51:1:740:C:H5'	1.44	0.83
15:O:93:ALA:HB1	15:O:96:VAL:HB	1.59	0.82
53:3:335:C:H2'	53:3:336:A:H8	1.44	0.82
27:b:38:LYS:HB2	51:1:692:C:H5''	1.59	0.82
51:1:161:A:H3'	51:1:162:U:H5''	1.62	0.82
52:2:3:C:H2'	52:2:4:C:H5''	1.62	0.82
58:B1:141:PHE:CE2	58:B1:296:LYS:HB2	2.15	0.81
53:3:1422:G:H2'	53:3:1423:G:C8	2.15	0.81
58:B1:144:TYR:HE1	58:B1:162:GLU:OE2	1.64	0.81
58:B1:141:PHE:HE2	58:B1:296:LYS:HB2	1.45	0.81
51:1:2107:G:H2'	51:1:2108:A:H8	1.44	0.81
53:3:405:U:H3'	53:3:406:G:H5'	1.61	0.81
58:B1:111:THR:HG23	58:B1:300:GLN:OE1	1.81	0.81
51:1:740:C:H42	51:1:757:G:H1	1.27	0.80
51:1:2553:G:H3'	51:1:2554:U:H5''	1.63	0.80
51:1:2156:G:H2'	51:1:2157:G:H5'	1.63	0.80
58:B1:37:GLU:O	58:B1:61:ILE:HD11	1.81	0.80
58:B1:770:LEU:HD13	59:B2:618:GLN:HG3	1.61	0.80
63:6:47:U:H2'	63:6:50:U:OP1	1.82	0.80
21:U:10:GLY:HA2	53:3:624:C:H4'	1.64	0.79
53:3:1088:G:H21	53:3:1167:A:H61	1.30	0.79
15:O:7:ARG:HB2	15:O:101:SER:HB2	1.62	0.79
36:l:17:LYS:HD2	51:1:663:G:H5''	1.62	0.79
52:2:88:C:H5''	52:2:89:U:OP1	1.82	0.78
53:3:112:G:H21	53:3:354:G:H5'	1.47	0.78
12:L:68:VAL:HG13	12:L:99:ALA:HB1	1.65	0.78
51:1:1064:C:H3'	51:1:1065:U:C5'	2.14	0.78
52:2:30:C:H2'	52:2:31:C:H5'	1.66	0.78
33:i:7:TYR:CE2	33:i:57:VAL:HB	2.16	0.77
38:n:4:ARG:HB2	51:1:2722:G:H4'	1.64	0.77
51:1:2128:G:H1	51:1:2160:C:N4	1.82	0.77
51:1:2799:A:H2'	51:1:2800:A:H5'	1.66	0.77
65:0:632:ILE:HD11	65:0:654:ILE:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:HG3	51:1:2884:U:H6	1.48	0.76
51:1:2656:U:H5''	65:0:146:ARG:NE	2.01	0.76
58:B1:186:GLN:HG3	58:B1:238:ILE:HG13	1.65	0.76
58:B1:202:ARG:HG2	58:B1:202:ARG:NH1	1.99	0.76
51:1:1020:A:H1'	51:1:1021:A:OP2	1.85	0.76
53:3:1012:A:H5'	53:3:1012:A:H8	1.48	0.76
51:1:974:G:H1'	51:1:975:A:C8	2.20	0.76
63:6:26:G:C2'	63:6:27:U:H5''	2.16	0.76
39:o:33:ARG:HB2	52:2:52:A:N6	2.00	0.75
53:3:769:G:H4'	53:3:1513:A:H4'	1.67	0.75
43:s:6:LYS:HG3	51:1:494:G:H4'	1.68	0.75
39:o:15:ARG:NH2	52:2:8:C:H5''	2.02	0.75
51:1:855:G:H2'	51:1:856:G:H5''	1.67	0.75
14:N:30:ASN:HD21	14:N:66:VAL:H	1.35	0.75
25:Y:55:PRO:HD3	53:3:193:C:H4'	1.69	0.75
51:1:760:G:H5'	51:1:760:G:H8	1.50	0.75
51:1:572:A:H61	51:1:2029:G:H21	1.35	0.75
15:O:41:PRO:HB3	53:3:1151:A:C1'	2.16	0.74
51:1:1326:U:H2'	51:1:1327:A:H8	1.51	0.74
51:1:694:U:OP1	51:1:1569:A:H1'	1.86	0.74
51:1:940:G:H2'	51:1:941:A:H5''	1.68	0.74
31:f:174:LYS:HD2	51:1:2529:G:H5'	1.68	0.74
58:B1:68:TYR:C	58:B1:75:TYR:CE2	2.65	0.74
18:R:105:ALA:HA	53:3:948:C:OP1	1.88	0.74
55:8:16:DT:P	58:B1:346:ARG:HH12	2.10	0.74
58:B1:110:PRO:HG2	58:B1:183:GLU:HG3	1.68	0.74
57:A2:66:HIS:HB3	59:B2:874:GLY:HA2	1.68	0.74
9:I:38:GLY:HA3	53:3:542:G:H5'	1.69	0.74
53:3:1028:C:H3'	53:3:1029:U:H5''	1.68	0.74
51:1:1062:G:OP1	51:1:1063:G:OP2	2.06	0.73
53:3:1421:G:H3'	53:3:1422:G:C4'	2.17	0.73
55:8:3:DC:H2'	55:8:4:DT:H72	1.69	0.73
56:9:27:DC:OP2	59:B2:542:ARG:NE	2.21	0.73
51:1:2163:A:H2'	51:1:2164:C:H5'	1.71	0.73
65:0:448:TRP:HB2	65:0:457:ILE:HB	1.70	0.73
1:A:64:PHE:CD1	53:3:1011:C:H4'	2.17	0.73
12:L:72:VAL:HG23	12:L:88:VAL:O	1.89	0.73
58:B1:157:GLN:OE1	58:B1:157:GLN:HA	1.88	0.73
58:B1:107:LEU:HD11	58:B1:242:LEU:HB2	1.70	0.73
58:B1:211:GLU:HG2	58:B1:215:LYS:HE3	1.71	0.73
58:B1:1143:ASP:OD1	58:B1:1148:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:6:44:A:H2'	63:6:45:G:C8	2.24	0.73
58:B1:142:GLU:HG3	58:B1:142:GLU:O	1.89	0.72
9:I:12:ARG:HG2	9:I:33:ILE:HA	1.71	0.72
51:1:2502:G:H5'	51:1:2503:A:H5''	1.69	0.72
53:3:352:C:H4'	53:3:354:G:OP1	1.89	0.72
33:i:10:LEU:CD1	51:1:1061:U:H1'	2.20	0.72
53:3:1088:G:N2	53:3:1167:A:H61	1.86	0.72
46:v:49:ASN:ND2	51:1:1040:A:H4'	2.05	0.72
51:1:1252:G:O2'	51:1:1253:A:H5''	1.90	0.72
58:B1:220:ARG:HG2	58:B1:220:ARG:HH11	1.55	0.72
31:f:70:LEU:HD11	51:1:2758:A:C2	2.25	0.72
47:w:38:GLY:HA2	51:1:2330:G:H21	1.52	0.72
33:i:130:GLY:HA3	51:1:1079:C:H1'	1.71	0.72
55:8:3:DC:C2'	55:8:4:DT:H72	2.19	0.72
58:B1:210:SER:HB3	58:B1:213:LYS:HB2	1.71	0.72
53:3:560:A:H5'	53:3:566:G:N2	2.05	0.71
37:m:12:MET:HA	51:1:910:A:H62	1.55	0.71
51:1:703:U:H2'	51:1:704:G:H5'	1.72	0.71
19:S:52:ARG:HH11	53:3:1317:C:H42	1.38	0.71
58:B1:105:ILE:HD12	58:B1:242:LEU:HD22	1.71	0.71
27:b:201:LEU:HD22	53:3:773:G:H5''	1.72	0.71
36:l:19:LEU:HD23	51:1:587:C:C2	2.25	0.71
39:o:55:GLU:HG2	52:2:116:G:H5'	1.72	0.71
51:1:2743:U:H2'	51:1:2744:G:H5''	1.72	0.71
33:i:79:LEU:HD21	33:i:132:ALA:HB2	1.71	0.71
51:1:718:A:H2'	51:1:719:C:O4'	1.91	0.71
51:1:2792:A:H2'	51:1:2793:C:H5''	1.72	0.71
53:3:1316:G:H2'	53:3:1317:C:H5''	1.73	0.71
51:1:414:C:H2'	51:1:415:A:H8	1.54	0.71
10:J:61:LYS:NZ	53:3:1073:U:OP2	2.24	0.70
14:N:70:GLY:HA3	53:3:1371:G:O3'	1.90	0.70
15:O:44:THR:HG23	53:3:1151:A:H5''	1.71	0.70
33:i:92:PRO:CB	51:1:1077:A:H1'	2.22	0.70
52:2:115:A:H2'	52:2:116:G:C8	2.26	0.70
53:3:1422:G:H2'	53:3:1423:G:H8	1.55	0.70
38:n:20:MET:HE2	51:1:1277:G:H5'	1.74	0.70
53:3:1218:C:H2'	53:3:1219:A:C8	2.27	0.70
51:1:2691:C:H2'	51:1:2692:G:C8	2.26	0.70
48:x:17:ARG:HG3	51:1:380:G:H5'	1.72	0.70
51:1:807:U:H2'	51:1:808:G:H8	1.55	0.70
51:1:876:C:H3'	51:1:877:A:H4'	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2634:A:H2'	51:1:2635:A:O4'	1.91	0.70
33:i:79:LEU:HD13	33:i:128:ILE:HG22	1.73	0.70
53:3:335:C:H2'	53:3:336:A:C8	2.26	0.70
55:8:17:DC:OP2	59:B2:1261:GLY:HA2	1.90	0.70
58:B1:128:LEU:HD11	58:B1:189:LEU:HG	1.73	0.70
4:D:34:ARG:HD3	51:1:467:G:OP2	1.91	0.70
51:1:663:G:C2'	51:1:664:G:H5''	2.20	0.70
53:3:78:A:H2'	53:3:79:G:O4'	1.91	0.70
33:i:92:PRO:CB	51:1:1077:A:C1'	2.70	0.70
53:3:1421:G:C8	53:3:1422:G:H1'	2.26	0.69
58:B1:352:ARG:HD2	59:B2:1268:GLN:HE22	1.55	0.69
66:h:6:5OH:N	66:h:6:5OH:HS	2.07	0.69
40:p:1:SER:H1	51:1:2875:C:H4'	1.57	0.69
40:p:59:THR:HG22	40:p:72:VAL:HG12	1.75	0.69
51:1:760:G:H2'	51:1:761:A:H5'	1.72	0.69
58:B1:93:THR:HB	58:B1:97:VAL:HG21	1.73	0.69
53:3:1513:A:H2'	53:3:1514:G:H8	1.58	0.69
51:1:2123:G:N7	51:1:2170:A:H4'	2.07	0.69
51:1:2296:U:H5''	51:1:2297:A:OP1	1.92	0.69
51:1:2566:A:H4'	51:1:2567:G:H5''	1.74	0.69
53:3:358:U:H2'	53:3:359:G:C8	2.28	0.69
53:3:483:C:H2'	53:3:484:G:C8	2.27	0.69
53:3:1293:C:H2'	53:3:1294:G:H8	1.58	0.69
58:B1:161:THR:HG22	58:B1:164:GLN:HB2	1.75	0.69
58:B1:832:LYS:C	58:B1:1242:ARG:HH12	2.01	0.69
51:1:2638:G:H1'	51:1:2778:A:H61	1.58	0.69
53:3:837:U:H2'	53:3:838:G:H8	1.57	0.69
35:k:48:PRO:HB3	53:3:1423:G:C5'	2.14	0.68
58:B1:289:ASP:CB	61:NG:104:SER:CB	2.71	0.68
14:N:35:GLU:HA	14:N:39:GLY:HA3	1.75	0.68
51:1:1063:G:H5''	51:1:1064:C:C6	2.28	0.68
59:B2:65:ASN:HB3	59:B2:105:TYR:HB2	1.73	0.68
39:o:12:THR:HB	51:1:2334:U:H5'	1.76	0.68
51:1:2691:C:H2'	51:1:2692:G:H8	1.58	0.68
52:2:3:C:C2'	52:2:4:C:H5''	2.23	0.68
7:G:46:VAL:HG23	7:G:47:PRO:HD3	1.75	0.68
28:c:13:ARG:HH11	51:1:2683:C:H4'	1.58	0.68
55:8:3:DC:C6	55:8:4:DT:H72	2.29	0.68
51:1:807:U:H2'	51:1:808:G:C8	2.28	0.68
58:B1:141:PHE:CD2	58:B1:293:ARG:O	2.47	0.68
62:5:47:U:H4'	62:5:48:C:H5'	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:ALA:HB1	53:3:407:U:H5''	1.75	0.68
32:g:8:LYS:HB2	32:g:15:LEU:HG	1.76	0.68
51:1:1098:A:C2'	51:1:1099:G:H5'	2.22	0.68
27:b:48:ILE:HG22	51:1:779:U:OP1	1.94	0.68
51:1:1869:G:H3'	51:1:1870:C:C5'	2.24	0.68
53:3:207:C:H2'	53:3:208:U:H5''	1.74	0.68
10:J:22:LYS:HG3	53:3:1081:A:H5'	1.75	0.68
58:B1:39:LYS:O	58:B1:273:ILE:CG2	2.41	0.68
58:B1:117:LEU:HD12	58:B1:117:LEU:O	1.94	0.68
66:h:4:SER:O	66:h:5:UAL:N1	2.26	0.68
58:B1:111:THR:CG2	58:B1:300:GLN:CD	2.66	0.67
58:B1:243:PRO:HG2	59:B2:1332:SER:O	1.93	0.67
58:B1:395:LYS:HZ2	58:B1:399:LYS:CD	2.07	0.67
65:0:515:TYR:HB3	65:0:584:HIS:CG	2.28	0.67
63:6:69:C:C2'	63:6:70:G:H5''	2.24	0.67
51:1:255:A:H2'	51:1:256:A:O4'	1.95	0.67
51:1:1550:C:H2'	51:1:1551:A:H8	1.60	0.67
34:j:30:THR:HG21	51:1:1012:U:O4	1.94	0.67
51:1:784:G:H5'	51:1:785:G:OP1	1.94	0.67
53:3:603:U:H2'	53:3:604:G:H8	1.58	0.67
58:B1:1355:ARG:NH1	58:B1:1369:ARG:HH12	1.93	0.67
14:N:83:THR:HG21	14:N:102:PHE:HB3	1.77	0.67
51:1:635:C:H2'	51:1:636:G:H8	1.58	0.67
51:1:1059:G:H3'	51:1:1060:U:H2'	1.77	0.67
13:M:28:SER:HB2	13:M:56:PRO:HB2	1.77	0.67
65:0:66:ALA:HB3	65:0:88:ASP:HB3	1.76	0.67
11:K:76:THR:HA	11:K:79:ARG:HG2	1.76	0.66
51:1:729:G:H4'	51:1:763:G:H5'	1.77	0.66
53:3:76:G:H2'	53:3:77:A:H5'	1.76	0.66
58:B1:108:ALA:HB3	58:B1:279:LEU:HD22	1.77	0.66
58:B1:978:ARG:HG2	58:B1:1197:ASN:HD21	1.60	0.66
14:N:4:GLN:HE22	53:3:1131:G:H5'	1.61	0.66
51:1:635:C:H2'	51:1:636:G:C8	2.30	0.66
55:8:12:DG:OP2	58:B1:339:ARG:NH1	2.27	0.66
55:8:23:DC:H2''	55:8:24:DC:C5	2.30	0.66
53:3:1333:A:H2'	53:3:1334:G:O4'	1.95	0.66
53:3:948:C:H5'	53:3:1306:A:O2'	1.95	0.66
51:1:1378:A:H1'	51:1:1379:U:C5	2.30	0.66
52:2:3:C:H42	52:2:117:G:H1	1.44	0.66
58:B1:984:LEU:HB3	58:B1:993:GLU:HB2	1.76	0.66
51:1:855:G:C2'	51:1:856:G:H5''	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:884:U:H4'	53:3:885:G:H5''	1.77	0.66
51:1:1297:C:OP1	51:1:2710:C:H4'	1.97	0.65
4:D:26:ASN:CG	51:1:682:G:H5'	2.21	0.65
17:Q:76:HIS:HB2	65:0:425:LYS:HD2	1.77	0.65
51:1:2383:G:O2'	51:1:2384:U:H5'	1.97	0.65
58:B1:193:ASP:HB3	58:B1:196:GLN:HB2	1.78	0.65
53:3:29:U:O2'	53:3:30:U:H5'	1.96	0.65
53:3:813:U:C2'	53:3:814:A:H5''	2.26	0.65
58:B1:108:ALA:CB	58:B1:279:LEU:HD22	2.25	0.65
58:B1:975:ILE:HG22	58:B1:977:SER:H	1.62	0.65
51:1:310:A:C2'	51:1:311:A:H5''	2.27	0.65
51:1:1752:C:H2'	51:1:1753:G:C8	2.31	0.65
51:1:414:C:H2'	51:1:415:A:C8	2.32	0.65
55:8:3:DC:C2'	55:8:4:DT:C7	2.75	0.65
65:0:558:GLN:HA	65:0:561:LEU:HD12	1.77	0.65
51:1:2177:C:O2'	64:a:170:ILE:HG21	1.97	0.65
53:3:663:A:H5'	53:3:836:G:OP1	1.95	0.65
58:B1:141:PHE:HD2	58:B1:293:ARG:O	1.80	0.65
51:1:2715:C:H3'	51:1:2716:C:H5''	1.79	0.65
58:B1:461:PHE:HD2	59:B2:813:GLU:HB2	1.61	0.65
9:I:101:VAL:HG13	9:I:106:PHE:HB2	1.79	0.65
36:l:20:GLY:HA2	36:l:28:GLY:HA2	1.79	0.65
52:2:95:U:H2'	52:2:96:G:H8	1.62	0.65
58:B1:1037:PHE:HB3	58:B1:1040:MET:HB2	1.78	0.65
58:B1:162:GLU:HA	58:B1:162:GLU:OE1	1.97	0.64
51:1:1752:C:H2'	51:1:1753:G:H8	1.62	0.64
53:3:1260:G:H4'	53:3:1284:C:H5'	1.80	0.64
8:H:78:LYS:HB2	8:H:81:GLU:HB3	1.79	0.64
51:1:1139:G:O2'	51:1:1140:C:H5'	1.98	0.64
58:B1:289:ASP:CG	61:NG:104:SER:CB	2.70	0.64
59:B2:1282:GLY:HA3	60:W0:17:PHE:HE1	1.63	0.64
51:1:310:A:H2'	51:1:311:A:H5''	1.79	0.64
53:3:664:G:H22	53:3:741:G:H1	1.45	0.64
59:B2:314:ASN:HD21	59:B2:348:SER:HA	1.62	0.64
23:W:42:ARG:NH2	53:3:721:G:C5'	2.51	0.64
43:s:42:LYS:HB2	51:1:2010:G:H5''	1.80	0.64
51:1:1827:U:H2'	51:1:1828:G:H5'	1.80	0.64
51:1:2808:G:H2'	51:1:2890:G:C6	2.32	0.64
51:1:855:G:C3'	51:1:856:G:H5''	2.28	0.64
51:1:1906:G:C3'	51:1:1907:G:H5''	2.27	0.64
51:1:151:C:H2'	51:1:152:A:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1012:A:H5'	53:3:1012:A:C8	2.31	0.64
53:3:1293:C:H2'	53:3:1294:G:C8	2.33	0.64
7:G:8:MET:HE3	7:G:46:VAL:HG11	1.79	0.63
8:H:125:ARG:HA	59:B2:905:ILE:CB	2.28	0.63
30:e:84:ILE:HG21	51:1:2312:U:H4'	1.80	0.63
51:1:1186:G:H2'	51:1:1187:G:O4'	1.97	0.63
52:2:3:C:C3'	52:2:4:C:H5''	2.27	0.63
53:3:971:G:H1'	53:3:1365:G:O2'	1.98	0.63
53:3:662:U:H2'	53:3:663:A:C8	2.33	0.63
58:B1:68:TYR:HB3	58:B1:75:TYR:CE2	2.32	0.63
39:o:100:HIS:NE2	52:2:48:U:H4'	2.13	0.63
53:3:1274:A:O2'	53:3:1275:A:H5''	1.98	0.63
2:B:5:ASN:ND2	51:1:2020:A:H62	1.96	0.63
2:B:49:ARG:HG3	51:1:2884:U:C6	2.32	0.63
51:1:876:C:H3'	51:1:877:A:O4'	1.99	0.63
53:3:1349:A:H2'	53:3:1350:A:O4'	1.98	0.63
58:B1:245:LEU:HG	58:B1:246:PRO:HD2	1.79	0.63
58:B1:289:ASP:OD2	61:NG:104:SER:CB	2.46	0.63
58:B1:918:ILE:HG22	59:B2:1280:ALA:HB1	1.79	0.63
65:0:632:ILE:HG23	65:0:642:LEU:HB3	1.80	0.63
33:i:123:ALA:HA	33:i:126:ARG:HD2	1.80	0.63
14:N:118:ARG:HH22	53:3:1233:G:H5'	1.62	0.63
33:i:92:PRO:HB2	51:1:1077:A:C1'	2.27	0.63
39:o:33:ARG:HB2	52:2:52:A:H62	1.62	0.63
14:N:118:ARG:NH2	53:3:1233:G:H5'	2.13	0.63
15:O:12:ALA:HB2	15:O:96:VAL:HG13	1.81	0.63
51:1:1960:A:H2'	51:1:1961:C:H5''	1.81	0.63
59:B2:120:GLN:NE2	59:B2:490:GLN:OE1	2.32	0.63
53:3:1513:A:H2'	53:3:1514:G:C8	2.33	0.63
58:B1:201:LEU:HB2	58:B1:221:ILE:HD13	1.80	0.63
28:c:35:THR:HG22	28:c:73:VAL:HG21	1.79	0.63
33:i:27:LEU:HD21	33:i:34:ILE:HB	1.79	0.63
35:k:5:GLN:HA	35:k:20:MET:HE3	1.80	0.63
35:k:66:LYS:NZ	35:k:80:ASP:O	2.32	0.63
43:s:11:ARG:HG3	51:1:1322:A:OP1	1.99	0.63
65:0:228:GLU:HB2	65:0:255:ARG:HH12	1.63	0.63
10:J:107:GLY:HA3	53:3:9:G:H5'	1.80	0.62
22:V:63:CYS:HG	22:V:73:THR:HG1	1.47	0.62
28:c:170:VAL:HG21	51:1:2679:A:H5'	1.81	0.62
53:3:79:G:O2'	53:3:80:A:H5'	1.98	0.62
53:3:1304:G:H2'	53:3:1305:G:H1'	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:105:ARG:HG3	53:3:1118:U:H5'	1.79	0.62
53:3:1073:U:H2'	53:3:1074:G:H8	1.64	0.62
27:b:144:GLU:HB2	27:b:187:CYS:HB3	1.81	0.62
35:k:76:VAL:H	40:p:72:VAL:HG22	1.63	0.62
51:1:2831:G:OP1	51:1:2834:G:H4'	1.99	0.62
19:S:48:GLN:HE22	24:X:11:ASP:HA	1.64	0.62
27:b:200:MET:HG3	51:1:1820:U:O2	2.00	0.62
33:i:10:LEU:HG	51:1:1061:U:H1'	1.81	0.62
40:p:2:ASN:HD21	51:1:2876:G:H4'	1.63	0.62
51:1:1078:U:H5''	51:1:1079:C:H5'	1.82	0.62
51:1:2682:A:N6	51:1:2728:U:H1'	2.02	0.62
53:3:583:A:H2'	53:3:584:G:O4'	1.99	0.62
53:3:1421:G:H3'	53:3:1422:G:C5'	2.30	0.62
53:3:1421:G:C3'	53:3:1422:G:H4'	2.26	0.62
51:1:1701:A:H2'	51:1:1702:G:H5'	1.81	0.62
53:3:545:C:O2'	53:3:549:C:H5''	2.00	0.62
58:B1:111:THR:CG2	58:B1:300:GLN:NE2	2.63	0.62
58:B1:1357:ILE:HD11	59:B2:1287:LEU:HD13	1.81	0.62
46:v:21:ARG:HH22	52:2:77:U:P	2.23	0.62
51:1:1533:C:H3'	51:1:1534:U:H5''	1.82	0.62
51:1:2248:C:H2'	51:1:2249:U:H5'	1.81	0.62
53:3:999:C:H2'	53:3:1000:A:H8	1.64	0.62
55:8:1:DC:H2''	55:8:2:DC:C5	2.35	0.62
31:f:70:LEU:HD11	51:1:2758:A:H2	1.64	0.62
51:1:1837:C:H2'	51:1:1899:A:H61	1.65	0.62
53:3:950:U:H2'	53:3:951:G:H8	1.65	0.62
33:i:9:LYS:NZ	51:1:1061:U:OP1	2.30	0.62
40:p:52:ARG:HH22	51:1:2720:U:P	2.23	0.62
51:1:2126:A:H2'	51:1:2162:G:H21	1.65	0.62
58:B1:1355:ARG:NH1	58:B1:1369:ARG:NH1	2.47	0.62
7:G:67:LEU:HD12	7:G:160:LEU:HD22	1.81	0.61
9:I:151:GLN:NE2	53:3:437:U:H5''	2.14	0.61
18:R:28:ARG:HH22	18:R:61:LYS:HB2	1.64	0.61
51:1:1655:A:C2	51:1:2049:G:H4'	2.35	0.61
53:3:999:C:H2'	53:3:1000:A:C8	2.35	0.61
21:U:11:ALA:HA	53:3:44:A:OP1	2.00	0.61
51:1:2185:U:H2'	51:1:2186:G:H8	1.65	0.61
53:3:1479:C:H2'	53:3:1480:A:H8	1.66	0.61
58:B1:100:GLU:HA	59:B2:1328:LYS:HE2	1.82	0.61
58:B1:750:PRO:CB	59:B2:549:ASP:OD2	2.45	0.61
10:J:75:LEU:HD22	10:J:119:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:116:GLY:N	53:3:1367:C:OP1	2.32	0.61
27:b:137:GLY:HA3	53:3:712:A:H5'	1.82	0.61
52:2:63:C:H2'	52:2:64:G:H8	1.64	0.61
58:B1:68:TYR:HB3	58:B1:75:TYR:CZ	2.35	0.61
4:D:21:ARG:NH1	51:1:466:A:H5'	2.14	0.61
8:H:18:ASN:ND2	19:S:89:ARG:O	2.33	0.61
51:1:1180:U:H3'	51:1:1181:U:H6	1.63	0.61
53:3:219:U:H2'	53:3:220:G:H8	1.65	0.61
53:3:768:A:OP1	53:3:804:U:H4'	2.01	0.61
53:3:1241:G:H2'	53:3:1242:G:H8	1.65	0.61
58:B1:288:PRO:HB3	61:NG:105:ASP:CB	2.30	0.61
58:B1:395:LYS:NZ	58:B1:399:LYS:HD3	2.15	0.61
58:B1:770:LEU:HD13	59:B2:618:GLN:CG	2.30	0.61
31:f:123:GLU:HG3	31:f:125:PRO:HD3	1.82	0.61
53:3:91:U:C3'	53:3:92:U:H5''	2.31	0.61
59:B2:528:ARG:NH2	59:B2:576:SER:O	2.30	0.61
53:3:130:A:H1'	53:3:264:C:H5'	1.82	0.61
53:3:1497:G:H2'	53:3:1498:U:H5'	1.82	0.61
58:B1:395:LYS:HZ2	58:B1:399:LYS:HD3	1.63	0.61
65:0:29:ARG:HD2	65:0:272:ASN:HD22	1.66	0.61
51:1:2128:G:P	64:a:38:PHE:HB3	2.41	0.61
53:3:622:A:H2'	53:3:623:C:H5'	1.83	0.61
58:B1:154:LEU:HD21	58:B1:160:LEU:HD21	1.83	0.61
58:B1:223:LEU:HG	58:B1:223:LEU:O	2.00	0.61
58:B1:1161:GLY:HA3	58:B1:1179:PRO:HA	1.83	0.61
33:i:89:SER:HB3	51:1:1063:G:C8	2.36	0.61
41:q:23:TYR:CD1	51:1:533:G:H5'	2.35	0.61
51:1:1097:U:H2'	51:1:1098:A:O4'	2.00	0.61
51:1:1807:G:H2'	51:1:1808:A:H5'	1.82	0.61
55:8:3:DC:H2'	55:8:4:DT:C7	2.30	0.61
19:S:7:ALA:HB1	53:3:995:C:H5'	1.83	0.60
29:d:53:THR:HG21	51:1:452:G:H8	1.66	0.60
51:1:2245:U:H5''	51:1:2246:G:H5'	1.83	0.60
53:3:530:G:H3'	53:3:531:U:C5'	2.31	0.60
53:3:651:C:H2'	53:3:652:U:C6	2.35	0.60
59:B2:55:SER:OG	59:B2:465:ARG:NH1	2.33	0.60
53:3:397:A:H3'	53:3:397:A:N3	2.16	0.60
58:B1:128:LEU:HA	58:B1:192:MET:HE1	1.81	0.60
64:a:50:ILE:HB	64:a:57:GLN:HB3	1.82	0.60
17:Q:30:ARG:HB3	53:3:363:A:OP2	2.00	0.60
17:Q:109:ARG:HB3	17:Q:118:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:49:ALA:HA	53:3:723:U:O4	2.00	0.60
32:g:43:ASN:HA	32:g:46:PHE:HB2	1.83	0.60
51:1:2128:G:H21	51:1:2173:A:H1'	1.66	0.60
51:1:2661:G:H5''	65:0:19:ILE:HD11	1.83	0.60
57:A1:38:THR:HB	57:A2:45:ARG:HD3	1.82	0.60
51:1:1827:U:C2'	51:1:1828:G:H5'	2.30	0.60
58:B1:633:ALA:HA	59:B2:806:PRO:O	2.01	0.60
58:B1:951:GLN:NE2	58:B1:1014:GLY:O	2.35	0.60
59:B2:1072:ASN:ND2	59:B2:1111:GLN:OE1	2.34	0.60
65:0:470:VAL:HG13	65:0:481:ALA:HB3	1.82	0.60
38:n:39:PRO:HG3	51:1:1651:G:H5'	1.82	0.60
46:v:9:ARG:HB3	46:v:41:GLU:HB2	1.83	0.60
53:3:1016:A:H4'	53:3:1218:C:H4'	1.83	0.60
11:K:3:HIS:HA	11:K:65:GLU:HA	1.81	0.60
18:R:27:THR:HG21	53:3:1328:C:H5''	1.83	0.60
51:1:1417:C:H4'	51:1:1587:G:H21	1.67	0.60
51:1:2267:A:H5''	51:1:2268:A:H5'	1.84	0.60
34:j:27:ARG:HD2	51:1:1143:A:H62	1.67	0.60
51:1:41:C:H2'	51:1:42:A:H5''	1.84	0.60
51:1:2061:G:H2'	51:1:2501:C:O2'	2.01	0.60
53:3:1060:U:H3	53:3:1197:A:H61	1.48	0.60
55:8:11:DC:H2'	55:8:12:DG:C8	2.37	0.60
57:A1:112:ALA:HB3	57:A1:126:PRO:HA	1.83	0.60
59:B2:69:GLN:HE21	59:B2:101:ARG:HD2	1.67	0.60
8:H:122:GLN:HB3	8:H:127:VAL:HG21	1.83	0.60
9:I:120:LYS:HB3	9:I:130:ASN:HB3	1.84	0.60
42:r:35:PHE:HB2	42:r:59:ILE:HB	1.83	0.60
53:3:1304:G:H2'	53:3:1305:G:C1'	2.31	0.60
6:F:4:ARG:HG2	51:1:2466:C:OP1	2.02	0.60
43:s:59:GLU:HB3	43:s:66:ILE:HD11	1.82	0.60
51:1:2183:A:H2'	51:1:2184:A:H5'	1.82	0.60
51:1:2220:U:H2'	51:1:2221:G:H8	1.67	0.60
58:B1:144:TYR:CE1	58:B1:162:GLU:OE2	2.51	0.60
28:c:135:GLY:HA2	51:1:743:A:OP1	2.02	0.60
40:p:102:ARG:NH2	51:1:1754:A:O3'	2.35	0.60
51:1:1906:G:H3'	51:1:1907:G:H5''	1.84	0.60
51:1:2343:U:H2'	51:1:2344:U:C6	2.37	0.60
52:2:11:C:H2'	52:2:12:C:O4'	2.02	0.60
57:A1:211:ILE:HG12	57:A1:219:ARG:HH12	1.65	0.60
58:B1:201:LEU:HD11	58:B1:220:ARG:HH11	1.67	0.60
58:B1:342:LEU:HD23	58:B1:1352:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:51:HIS:HA	24:X:56:HIS:HA	1.83	0.59
53:3:1530:G:H2'	53:3:1531:A:C8	2.36	0.59
58:B1:514:THR:HG21	58:B1:596:LEU:HD12	1.84	0.59
59:B2:918:LEU:O	59:B2:918:LEU:HD23	2.02	0.59
51:1:2371:G:O2'	51:1:2372:U:H5'	2.02	0.59
52:2:104:A:H2'	52:2:105:G:O4'	2.02	0.59
53:3:91:U:H3'	53:3:92:U:H5''	1.84	0.59
33:i:75:ALA:HB3	51:1:1060:U:OP1	2.02	0.59
51:1:1064:C:C3'	51:1:1065:U:H5''	2.24	0.59
53:3:1241:G:H2'	53:3:1242:G:C8	2.36	0.59
55:8:7:DC:H2''	55:8:8:DT:H71	1.84	0.59
6:F:2:LYS:NZ	6:F:32:LYS:O	2.35	0.59
50:z:12:ALA:HB1	50:z:20:LYS:HG2	1.83	0.59
52:2:95:U:H2'	52:2:96:G:C8	2.37	0.59
64:a:28:ALA:HA	64:a:31:LYS:HD3	1.85	0.59
8:H:106:ARG:HG3	8:H:107:LYS:HG3	1.84	0.59
9:I:37:PRO:HD2	9:I:41:GLY:HA3	1.83	0.59
51:1:629:G:H5''	51:1:650:C:O2'	2.03	0.59
51:1:1068:G:N3	51:1:1096:A:H5'	2.17	0.59
51:1:2107:G:H2'	51:1:2108:A:C8	2.32	0.59
53:3:1326:U:H2'	53:3:1327:C:C6	2.37	0.59
55:8:11:DC:H5''	58:B1:1326:GLN:HB3	1.85	0.59
9:I:149:LYS:HG2	9:I:150:LYS:HG3	1.83	0.59
51:1:869:G:H1	51:1:908:C:H42	1.50	0.59
51:1:937:C:H2'	51:1:938:G:C8	2.38	0.59
51:1:1095:A:C2	65:0:632:ILE:HD13	2.38	0.59
53:3:210:C:H5'	53:3:211:G:C2	2.37	0.59
53:3:328:C:H4'	53:3:329:A:H5'	1.84	0.59
53:3:1218:C:H2'	53:3:1219:A:H8	1.67	0.59
14:N:8:THR:OG1	14:N:9:GLY:N	2.36	0.59
27:b:228:ASP:CG	51:1:780:G:H1	2.10	0.59
53:3:1275:A:H2'	53:3:1276:G:O4'	2.03	0.59
58:B1:97:VAL:HG11	58:B1:101:ARG:NH2	2.18	0.59
62:5:26:A:H61	62:5:44:G:H22	1.50	0.59
65:0:415:VAL:HB	65:0:416:ILE:HD12	1.84	0.59
6:F:11:CYS:SG	6:F:14:CYS:N	2.75	0.59
28:c:56:LYS:HE3	51:1:2830:C:H5''	1.85	0.59
51:1:1095:A:N3	65:0:632:ILE:HG21	2.18	0.59
51:1:1697:G:C3'	51:1:1698:A:H5''	2.31	0.59
53:3:936:C:H2'	53:3:937:A:O4'	2.02	0.59
53:3:1352:C:H2'	53:3:1353:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:ALA:HB2	53:3:499:A:N6	2.18	0.59
20:T:22:GLY:O	20:T:27:GLN:NE2	2.35	0.59
51:1:96:C:H2'	51:1:97:C:H6	1.68	0.59
51:1:876:C:C3'	51:1:877:A:H4'	2.32	0.59
51:1:2715:C:C3'	51:1:2716:C:H5''	2.33	0.59
53:3:123:U:H5''	53:3:311:C:O2'	2.03	0.59
53:3:381:C:H2'	53:3:382:A:O4'	2.02	0.59
56:9:12:DC:H3'	58:B1:47:ARG:HH12	1.68	0.59
58:B1:161:THR:HG23	58:B1:164:GLN:H	1.68	0.59
58:B1:638:SER:OG	58:B1:639:VAL:N	2.36	0.59
20:T:68:TYR:HB2	53:3:754:C:H4'	1.84	0.59
30:e:38:GLY:HA3	51:1:2312:U:O2	2.03	0.59
51:1:1509:A:H2'	51:1:1510:G:C8	2.38	0.59
58:B1:370:LYS:HG2	58:B1:441:LEU:HD23	1.84	0.59
20:T:23:SER:HA	53:3:751:U:H4'	1.85	0.58
32:g:55:GLU:HA	32:g:58:LEU:HB2	1.85	0.58
40:p:91:VAL:HG11	40:p:96:LEU:HD21	1.85	0.58
51:1:572:A:H61	51:1:2029:G:N2	2.00	0.58
58:B1:438:GLU:HG3	58:B1:485:MET:HE1	1.85	0.58
15:O:8:ILE:HB	15:O:74:VAL:HB	1.85	0.58
26:Z:39:LYS:NZ	53:3:1530:G:O6	2.37	0.58
51:1:1434:A:H2'	51:1:1435:G:C8	2.38	0.58
51:1:2663:G:OP1	65:0:59:ARG:HD3	2.02	0.58
52:2:3:C:H3'	52:2:4:C:H5''	1.85	0.58
53:3:358:U:H2'	53:3:359:G:H8	1.66	0.58
58:B1:725:MET:SD	59:B2:1101:LEU:HD23	2.42	0.58
59:B2:1142:ARG:NH1	59:B2:1161:LEU:O	2.36	0.58
53:3:410:G:H2'	53:3:429:U:C4	2.38	0.58
53:3:1395:C:C6	53:3:1395:C:H5'	2.38	0.58
58:B1:412:LEU:HD22	58:B1:441:LEU:HD21	1.84	0.58
16:P:23:HIS:HB3	16:P:30:ILE:HG23	1.85	0.58
23:W:28:LEU:HD21	23:W:58:ILE:HG12	1.85	0.58
33:i:120:ASP:HB3	33:i:123:ALA:HB3	1.84	0.58
33:i:126:ARG:HA	33:i:129:GLU:HG3	1.86	0.58
48:x:25:LYS:HE2	51:1:189:G:OP2	2.03	0.58
51:1:1443:U:H2'	51:1:1444:G:C8	2.38	0.58
58:B1:275:ARG:NH1	58:B1:278:ARG:NH1	2.51	0.58
59:B2:707:ALA:O	59:B2:711:ASP:HB2	2.03	0.58
47:w:20:LYS:HG3	51:1:2355:G:H4'	1.85	0.58
51:1:1810:A:H2'	51:1:1811:G:O4'	2.04	0.58
51:1:1846:G:H2'	51:1:1847:A:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2138:G:H2'	51:1:2139:U:H5'	1.84	0.58
53:3:76:G:C2'	53:3:77:A:H5'	2.34	0.58
58:B1:926:PRO:HG2	58:B1:1248:ILE:HD11	1.84	0.58
37:m:125:PRO:HB3	51:1:2485:G:O3'	2.04	0.58
51:1:472:A:H2'	51:1:473:G:H5'	1.86	0.58
53:3:670:G:H2'	53:3:671:G:H5''	1.86	0.58
65:0:515:TYR:HB3	65:0:584:HIS:HB2	1.86	0.58
8:H:123:LEU:HD21	8:H:129:PHE:HB3	1.85	0.58
27:b:79:ARG:NH1	27:b:81:GLU:OE2	2.36	0.58
36:l:126:ARG:NH1	51:1:635:C:OP2	2.37	0.58
42:r:61:ALA:HB2	42:r:98:ILE:HD13	1.86	0.58
51:1:2650:U:H2'	51:1:2651:C:C6	2.38	0.58
53:3:427:U:H2'	53:3:428:G:C8	2.39	0.58
55:8:16:DT:OP1	58:B1:346:ARG:NH1	2.37	0.58
33:i:10:LEU:CG	51:1:1061:U:H1'	2.34	0.58
34:j:27:ARG:NE	51:1:1143:A:N7	2.46	0.58
51:1:940:G:C2'	51:1:941:A:H5''	2.34	0.58
53:3:132:C:H5'	53:3:262:A:O2'	2.03	0.58
25:Y:55:PRO:HB3	53:3:193:C:O3'	2.04	0.58
51:1:1783:A:H5'	51:1:2608:G:H4'	1.86	0.58
57:A2:82:LEU:HD11	57:A2:171:LEU:HD23	1.86	0.58
58:B1:99:ARG:NH1	58:B1:99:ARG:HG3	2.17	0.58
4:D:9:VAL:HG12	51:1:1309:G:OP1	2.03	0.58
8:H:162:ALA:HB2	53:3:1056:U:H5'	1.85	0.58
29:d:163:ASN:HD21	51:1:322:A:H2'	1.68	0.58
39:o:10:ARG:HD2	51:1:2294:G:P	2.44	0.58
51:1:703:U:C2'	51:1:704:G:H5'	2.33	0.58
51:1:917:A:H5''	51:1:2268:A:H61	1.69	0.58
51:1:2469:A:H8	51:1:2469:A:H5'	1.69	0.58
53:3:813:U:H2'	53:3:814:A:C5'	2.32	0.58
53:3:837:U:H2'	53:3:838:G:C8	2.38	0.58
55:8:13:DT:H71	58:B1:791:ALA:HB2	1.85	0.58
1:A:64:PHE:HA	53:3:1011:C:C5'	2.33	0.57
3:C:44:GLN:OE1	51:1:2371:G:H4'	2.04	0.57
17:Q:28:GLN:HE22	53:3:33:A:H2	1.51	0.57
38:n:64:ARG:HH22	51:1:2852:G:H5'	1.68	0.57
52:2:118:C:H2'	52:2:119:A:H4'	1.86	0.57
53:3:1395:C:H5'	53:3:1395:C:H6	1.69	0.57
9:I:131:ILE:HD13	53:3:620:C:N3	2.18	0.57
42:r:6:GLN:HG2	42:r:11:GLN:HG2	1.84	0.57
51:1:553:G:H2'	51:1:554:U:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:729:G:H4'	51:1:763:G:C5'	2.34	0.57
51:1:748:G:O2'	51:1:749:A:H3'	2.03	0.57
53:3:70:U:H5''	53:3:71:A:OP1	2.03	0.57
58:B1:1361:THR:HB	59:B2:1284:ALA:HB3	1.85	0.57
8:H:174:LEU:HB2	53:3:1108:G:OP1	2.04	0.57
30:e:3:LEU:HA	30:e:6:TYR:HB3	1.86	0.57
30:e:41:GLU:HG3	30:e:44:ALA:HB3	1.86	0.57
43:s:18:ARG:NH1	43:s:76:VAL:O	2.37	0.57
51:1:760:G:H2'	51:1:761:A:C5'	2.35	0.57
51:1:2151:U:H2'	51:1:2152:G:C8	2.39	0.57
53:3:219:U:H2'	53:3:220:G:C8	2.38	0.57
58:B1:1046:ILE:HD12	58:B1:1059:LEU:HB3	1.86	0.57
14:N:54:VAL:HG11	14:N:93:LEU:HD23	1.86	0.57
18:R:97:ARG:HH12	53:3:1308:U:H5	1.52	0.57
36:l:30:THR:HG22	51:1:810:U:O4	2.04	0.57
51:1:1058:U:H5	51:1:1080:A:H61	1.50	0.57
51:1:2248:C:C2'	51:1:2249:U:H5'	2.35	0.57
51:1:2584:U:H2'	51:1:2585:U:H2'	1.86	0.57
53:3:1060:U:H2'	53:3:1061:G:H8	1.68	0.57
47:w:38:GLY:HA2	51:1:2330:G:N2	2.19	0.57
51:1:832:U:H2'	51:1:833:A:C8	2.39	0.57
51:1:1111:A:C2	51:1:1112:G:H1'	2.39	0.57
51:1:2117:A:H61	51:1:2170:A:H61	1.53	0.57
51:1:2398:U:H2'	51:1:2399:G:C8	2.39	0.57
53:3:1014:A:C2	53:3:1219:A:H1'	2.40	0.57
53:3:1404:C:H2'	53:3:1405:G:C8	2.40	0.57
22:V:67:SER:OG	22:V:68:LYS:N	2.37	0.57
51:1:1386:C:H2'	51:1:1387:A:H8	1.69	0.57
51:1:2124:G:H2'	51:1:2125:G:O4'	2.05	0.57
58:B1:741:ALA:O	58:B1:762:ASN:ND2	2.38	0.57
28:c:156:PHE:HB3	34:j:81:ILE:HG22	1.85	0.57
51:1:1801:A:H5''	51:1:2203:U:H2'	1.87	0.57
51:1:2757:A:H2'	51:1:2758:A:H5''	1.87	0.57
65:0:492:GLU:HB2	65:0:571:VAL:HG22	1.85	0.57
19:S:52:ARG:HG3	53:3:1317:C:N3	2.20	0.57
21:U:40:ASN:HB3	21:U:43:ALA:HB2	1.87	0.57
51:1:32:C:H2'	51:1:33:C:C6	2.40	0.57
51:1:1458:U:H4'	51:1:1459:G:C4	2.40	0.57
51:1:2743:U:H2'	51:1:2744:G:C5'	2.35	0.57
53:3:57:G:H5'	65:0:373:GLU:OE2	2.05	0.57
58:B1:37:GLU:O	58:B1:61:ILE:CD1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:615:LYS:HG2	60:W0:5:THR:HG21	1.85	0.57
51:1:668:A:H2'	51:1:670:A:H62	1.70	0.57
51:1:1109:C:H2'	51:1:1110:G:O4'	2.04	0.57
51:1:2514:U:H2'	51:1:2515:C:C6	2.40	0.57
51:1:2732:G:O2'	51:1:2733:A:H5'	2.05	0.57
58:B1:198:CYS:HA	58:B1:221:ILE:HD11	1.86	0.57
9:I:7:LYS:HE2	53:3:408:A:OP2	2.04	0.57
14:N:86:LEU:HB3	14:N:93:LEU:HD13	1.86	0.57
33:i:4:VAL:HA	33:i:7:TYR:HB3	1.87	0.57
16:P:51:PHE:HB3	16:P:55:ARG:HG3	1.86	0.56
51:1:1506:U:H2'	51:1:1507:C:C6	2.40	0.56
51:1:1775:U:H2'	51:1:1776:G:O4'	2.05	0.56
51:1:1893:C:H2'	51:1:1894:C:H5'	1.87	0.56
53:3:1201:A:H4'	53:3:1202:U:H5''	1.86	0.56
58:B1:99:ARG:CG	58:B1:99:ARG:HH11	2.18	0.56
59:B2:1122:LYS:NZ	59:B2:1126:ASP:OD1	2.38	0.56
25:Y:79:THR:HG21	53:3:187:G:H5'	1.86	0.56
36:l:2:ARG:NH1	36:l:5:THR:OG1	2.39	0.56
51:1:2127:G:O3'	64:a:38:PHE:HB3	2.05	0.56
51:1:2156:G:C2'	51:1:2157:G:H5'	2.34	0.56
58:B1:510:LEU:HD22	58:B1:601:ILE:HD12	1.86	0.56
25:Y:73:ARG:CZ	53:3:261:U:H5	2.18	0.56
28:c:146:ILE:HG12	51:1:2051:A:H4'	1.87	0.56
35:k:63:VAL:HG12	35:k:107:LEU:HD21	1.87	0.56
51:1:11:C:H2'	51:1:12:U:H5''	1.87	0.56
51:1:151:C:H2'	51:1:152:A:C8	2.40	0.56
51:1:1133:A:H4'	51:1:1134:A:H5''	1.87	0.56
53:3:280:C:H5''	53:3:281:G:OP2	2.04	0.56
53:3:458:U:H2'	53:3:459:A:C8	2.40	0.56
58:B1:247:PRO:HA	58:B1:250:ARG:HG3	1.87	0.56
6:F:23:ILE:HD13	51:1:1032:A:H1'	1.87	0.56
14:N:27:ILE:HG23	14:N:62:LEU:HB2	1.87	0.56
22:V:15:LYS:HB2	53:3:275:G:H5'	1.87	0.56
51:1:1318:U:H2'	51:1:1319:C:C6	2.40	0.56
51:1:1638:C:H4'	51:1:2710:C:O2	2.06	0.56
51:1:2556:C:H2'	51:1:2557:G:O4'	2.05	0.56
53:3:235:C:H2'	53:3:236:A:H8	1.69	0.56
53:3:427:U:H5''	53:3:542:G:OP1	2.06	0.56
53:3:1305:G:H22	53:3:1331:G:H2'	1.69	0.56
59:B2:818:VAL:HG22	59:B2:1096:ILE:HG12	1.87	0.56
59:B2:1142:ARG:NH2	59:B2:1166:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:94:ALA:C	15:O:96:VAL:H	2.13	0.56
29:d:27:LEU:HD13	51:1:600:G:H5'	1.88	0.56
40:p:47:ILE:HD11	40:p:61:ARG:HB3	1.88	0.56
51:1:1287:A:C2	51:1:1649:G:H4'	2.40	0.56
51:1:1550:C:H2'	51:1:1551:A:C8	2.40	0.56
51:1:2403:C:O2'	51:1:2404:U:H5'	2.05	0.56
52:2:97:C:C2'	52:2:98:G:H5'	2.35	0.56
12:L:115:MET:HA	12:L:118:ARG:HE	1.70	0.56
51:1:2682:A:H61	51:1:2728:U:C1'	2.06	0.56
53:3:1073:U:H2'	53:3:1074:G:C8	2.40	0.56
58:B1:102:MET:HG2	58:B1:246:PRO:HG3	1.87	0.56
59:B2:839:VAL:HG12	59:B2:1049:ILE:HG12	1.87	0.56
10:J:80:LEU:HB2	10:J:97:PRO:HB3	1.87	0.56
51:1:2167:U:H3	51:1:2170:A:N6	2.03	0.56
58:B1:241:VAL:O	58:B1:241:VAL:HG12	2.04	0.56
65:0:107:ASP:OD2	65:0:337:ARG:NH2	2.39	0.56
11:K:38:ARG:HH21	11:K:61:LEU:HD23	1.69	0.56
16:P:63:GLN:HG2	16:P:98:ALA:HB2	1.87	0.56
33:i:10:LEU:HD12	51:1:1061:U:H1'	1.86	0.56
51:1:1062:G:O2'	51:1:1063:G:H4'	2.05	0.56
53:3:1268:G:N2	53:3:1327:C:H1'	2.21	0.56
58:B1:508:LEU:HD22	59:B2:1101:LEU:HD21	1.88	0.56
40:p:91:VAL:HG21	40:p:96:LEU:HD11	1.87	0.56
51:1:760:G:H5'	51:1:760:G:C8	2.37	0.56
51:1:967:U:H2'	51:1:968:C:C6	2.41	0.56
51:1:972:A:OP2	51:1:974:G:H5'	2.06	0.56
51:1:2183:A:C2'	51:1:2184:A:H5'	2.36	0.56
58:B1:130:MET:HE2	58:B1:135:ILE:HG12	1.87	0.56
58:B1:1166:GLY:HA3	58:B1:1174:ARG:HB2	1.88	0.56
27:b:47:ARG:HD3	51:1:778:G:H5''	1.87	0.56
47:w:12:SER:HB3	51:1:2261:C:C5	2.41	0.56
51:1:2660:A:H2'	51:1:2661:G:O4'	2.05	0.56
53:3:603:U:H2'	53:3:604:G:C8	2.40	0.56
58:B1:160:LEU:HD22	58:B1:164:GLN:HB3	1.86	0.56
3:C:7:LYS:HA	3:C:23:THR:HA	1.88	0.55
33:i:78:LEU:HG	33:i:108:ILE:HD12	1.88	0.55
34:j:65:THR:OG1	51:1:1141:U:OP2	2.22	0.55
58:B1:1175:LEU:HD22	58:B1:1190:ILE:HD11	1.88	0.55
8:H:161:ILE:HG22	53:3:1196:A:N1	2.22	0.55
12:L:36:SER:HB2	14:N:42:THR:HG22	1.87	0.55
51:1:1558:C:H4'	51:1:1559:U:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1909:C:H2'	51:1:1910:G:C8	2.42	0.55
52:2:49:C:H2'	52:2:50:A:H8	1.70	0.55
58:B1:352:ARG:HD2	59:B2:1268:GLN:HE21	1.68	0.55
59:B2:13:LYS:HB2	59:B2:1180:MET:HE2	1.86	0.55
2:B:9:ARG:HG3	51:1:17:G:OP1	2.06	0.55
27:b:70:LYS:NZ	27:b:97:ASP:OD2	2.39	0.55
48:x:30:PRO:HG2	48:x:32:LEU:HD22	1.87	0.55
51:1:296:U:H2'	51:1:297:G:C8	2.40	0.55
51:1:322:A:H5'	51:1:340:A:H1'	1.88	0.55
51:1:1063:G:H5''	51:1:1064:C:H6	1.69	0.55
51:1:1557:C:C3'	51:1:1558:C:H5''	2.28	0.55
51:1:2113:U:H2'	51:1:2114:A:C8	2.40	0.55
51:1:2169:A:H2'	51:1:2170:A:O4'	2.06	0.55
51:1:2792:A:C2'	51:1:2793:C:H5''	2.36	0.55
53:3:82:G:H2'	53:3:83:C:H5'	1.88	0.55
53:3:211:G:H2'	53:3:212:G:H5'	1.88	0.55
10:J:54:GLU:HG3	10:J:56:PRO:HD2	1.89	0.55
18:R:89:ARG:HB2	18:R:96:VAL:HG12	1.88	0.55
22:V:67:SER:HB3	22:V:70:LYS:HB2	1.87	0.55
35:k:38:ILE:HG22	35:k:61:VAL:HB	1.88	0.55
51:1:1386:C:H2'	51:1:1387:A:C8	2.42	0.55
51:1:1794:A:H2'	51:1:1795:C:C6	2.41	0.55
53:3:570:G:H5'	53:3:820:U:O4'	2.07	0.55
53:3:950:U:H2'	53:3:951:G:C8	2.41	0.55
53:3:994:A:H3'	53:3:994:A:OP2	2.06	0.55
58:B1:42:GLU:HB3	58:B1:52:GLU:HG3	1.86	0.55
13:M:19:ALA:HB2	53:3:827:U:O2'	2.07	0.55
13:M:52:GLY:HA3	13:M:56:PRO:HA	1.88	0.55
26:Z:66:ARG:HH21	53:3:1099:G:H4'	1.70	0.55
50:z:37:ARG:NH2	51:1:929:U:H4'	2.21	0.55
51:1:1877:A:H2'	51:1:1878:G:O4'	2.07	0.55
53:3:918:A:H2'	53:3:919:A:O4'	2.06	0.55
7:G:45:THR:HG22	7:G:200:PRO:HB2	1.88	0.55
14:N:4:GLN:NE2	53:3:1131:G:H5'	2.22	0.55
16:P:126:ARG:NH2	53:3:796:C:O3'	2.39	0.55
51:1:1258:U:H2'	51:1:1259:G:C8	2.42	0.55
53:3:169:C:H2'	53:3:170:U:C6	2.42	0.55
58:B1:39:LYS:O	58:B1:273:ILE:HG21	2.06	0.55
59:B2:917:SER:O	59:B2:919:ARG:HG3	2.07	0.55
59:B2:985:GLU:HB3	59:B2:988:LYS:HB2	1.88	0.55
15:O:25:ILE:HD11	15:O:87:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:59:LYS:HD2	53:3:972:C:O3'	2.07	0.55
24:X:38:THR:HA	24:X:69:LYS:HA	1.89	0.55
33:i:105:LEU:HA	33:i:108:ILE:HG12	1.89	0.55
51:1:760:G:C2'	51:1:761:A:H5'	2.36	0.55
58:B1:144:TYR:HE1	58:B1:162:GLU:CD	2.14	0.55
58:B1:804:ALA:HA	58:B1:1259:GLN:HG3	1.88	0.55
59:B2:633:LEU:HD13	59:B2:644:LEU:HD23	1.89	0.55
19:S:58:ARG:NH1	53:3:979:C:O2	2.39	0.55
25:Y:81:GLN:HA	25:Y:84:LYS:HE3	1.87	0.55
51:1:1790:C:H2'	51:1:1791:A:C5	2.42	0.55
51:1:2800:A:H3'	51:1:2801:G:H5'	1.89	0.55
52:2:30:C:C2'	52:2:31:C:H5'	2.33	0.55
58:B1:759:ILE:HG23	58:B1:771:GLN:HB3	1.89	0.55
58:B1:833:GLU:HB2	58:B1:1242:ARG:NH1	2.22	0.55
1:A:64:PHE:HB2	53:3:1012:A:OP1	2.07	0.55
36:l:25:SER:HA	51:1:813:U:O4	2.07	0.55
51:1:1437:C:H2'	51:1:1438:U:C6	2.41	0.55
52:2:97:C:H2'	52:2:98:G:H5'	1.87	0.55
58:B1:58:CYS:SG	58:B1:59:ALA:N	2.80	0.55
51:1:814:C:C1'	51:1:1225:G:H21	2.06	0.55
52:2:63:C:H2'	52:2:64:G:C8	2.41	0.55
53:3:1280:A:O2'	53:3:1281:C:H5'	2.07	0.55
58:B1:800:LEU:HB3	58:B1:920:ALA:HB1	1.89	0.55
59:B2:360:LEU:HD13	59:B2:378:ARG:HH11	1.72	0.55
25:Y:4:LYS:HE2	53:3:332:G:OP1	2.06	0.54
40:p:94:ALA:HB2	51:1:2848:G:C8	2.42	0.54
51:1:1159:U:H2'	51:1:1160:G:H8	1.71	0.54
51:1:2151:U:H2'	51:1:2152:G:H8	1.73	0.54
51:1:2389:G:H5''	51:1:2390:U:O4'	2.08	0.54
51:1:2602:A:H4'	51:1:2603:G:H5'	1.90	0.54
22:V:45:VAL:HG22	22:V:72:TRP:HB2	1.90	0.54
32:g:1:MET:N	32:g:21:VAL:O	2.41	0.54
34:j:125:TYR:HH	34:j:132:HIS:HE2	1.55	0.54
51:1:96:C:H2'	51:1:97:C:C6	2.41	0.54
51:1:2636:C:H2'	51:1:2637:U:C6	2.42	0.54
21:U:18:GLN:HA	21:U:38:PHE:HA	1.90	0.54
24:X:77:ARG:HH22	53:3:1322:C:P	2.30	0.54
27:b:137:GLY:O	27:b:162:GLN:NE2	2.39	0.54
35:k:3:GLN:HE21	51:1:1666:G:H1'	1.72	0.54
35:k:48:PRO:CB	53:3:1423:G:H5''	2.16	0.54
51:1:1909:C:H2'	51:1:1910:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2428:G:H5''	51:1:2429:G:O5'	2.08	0.54
53:3:5:U:H4'	53:3:6:G:N7	2.23	0.54
53:3:1379:G:O2'	53:3:1380:U:H5'	2.07	0.54
64:a:33:LEU:HD22	64:a:216:THR:HB	1.89	0.54
65:0:617:MET:HE2	65:0:682:MET:HE3	1.89	0.54
8:H:45:GLU:HB3	8:H:46:LEU:HD12	1.89	0.54
11:K:10:VAL:HG12	11:K:84:VAL:HG12	1.88	0.54
27:b:235:GLU:HG2	51:1:2599:G:C8	2.42	0.54
44:t:15:HIS:HE1	51:1:1339:G:OP2	1.91	0.54
51:1:296:U:H2'	51:1:297:G:H8	1.71	0.54
51:1:644:A:H2'	51:1:645:C:H5''	1.89	0.54
51:1:1564:C:H2'	51:1:1565:C:O4'	2.08	0.54
52:2:115:A:H2'	52:2:116:G:H8	1.72	0.54
8:H:171:ARG:HG2	53:3:1106:G:H5''	1.90	0.54
14:N:17:ARG:HH12	53:3:1129:C:C5'	2.21	0.54
24:X:49:ALA:HA	24:X:58:PRO:HA	1.89	0.54
30:e:25:MET:HG2	52:2:57:A:C6	2.42	0.54
34:j:27:ARG:NH2	51:1:1142:A:H4'	2.11	0.54
48:x:16:ASN:ND2	51:1:2081:U:H5''	2.23	0.54
51:1:1045:C:H5'	51:1:1046:A:N7	2.21	0.54
51:1:1095:A:H1'	65:0:632:ILE:HG22	1.89	0.54
51:1:2026:U:H2'	51:1:2027:G:O4'	2.06	0.54
51:1:2215:C:H2'	51:1:2216:G:C8	2.43	0.54
53:3:256:U:H2'	53:3:257:G:C8	2.43	0.54
59:B2:103:VAL:HB	59:B2:114:VAL:HG11	1.89	0.54
63:6:19:G:H1'	63:6:57:A:C2	2.43	0.54
65:0:164:ALA:HB1	65:0:262:ILE:HD11	1.89	0.54
4:D:4:THR:O	51:1:687:C:H5''	2.07	0.54
15:O:10:LEU:HB2	15:O:72:ARG:HB2	1.88	0.54
42:r:14:VAL:HG21	42:r:98:ILE:HG13	1.88	0.54
51:1:2122:U:H2'	51:1:2123:G:C4'	2.38	0.54
53:3:575:G:O2'	53:3:821:G:H5'	2.08	0.54
58:B1:145:VAL:HG23	58:B1:159:ILE:HG22	1.89	0.54
7:G:175:ALA:HB1	7:G:180:ILE:HB	1.90	0.54
24:X:5:LYS:HG2	53:3:1313:U:OP2	2.07	0.54
45:u:11:ILE:HG13	45:u:21:ARG:HB3	1.90	0.54
51:1:918:A:H5''	52:2:97:C:O2'	2.07	0.54
52:2:29:A:H2'	52:2:30:C:C6	2.43	0.54
53:3:1342:C:H2'	53:3:1343:G:H8	1.73	0.54
59:B2:29:SER:O	59:B2:33:ASP:HB2	2.07	0.54
63:6:48:C:H5'	63:6:50:U:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:131:THR:HG22	33:i:135:MET:HE2	1.88	0.54
43:s:60:HIS:ND1	43:s:61:ASN:OD1	2.41	0.54
46:v:47:VAL:HA	46:v:50:MET:HG2	1.89	0.54
51:1:320:A:H4'	51:1:322:A:N7	2.23	0.54
51:1:554:U:H2'	51:1:555:G:O4'	2.08	0.54
51:1:995:C:H6	51:1:995:C:H5'	1.72	0.54
58:B1:785:ASP:O	58:B1:789:LYS:HB2	2.08	0.54
58:B1:799:ARG:HG2	58:B1:1325:PHE:HZ	1.72	0.54
10:J:141:ASP:O	10:J:145:ASN:ND2	2.40	0.54
30:e:37:MET:HB2	30:e:56:LEU:HD11	1.90	0.54
40:p:96:LEU:HB3	40:p:99:LEU:HD13	1.90	0.54
51:1:226:A:H5''	51:1:257:C:O2'	2.08	0.54
51:1:740:C:H5'	51:1:740:C:C6	2.34	0.54
51:1:1753:G:N2	51:1:1755:A:H3'	2.23	0.54
51:1:2398:U:H2'	51:1:2399:G:H8	1.72	0.54
53:3:231:U:H2'	53:3:232:G:H8	1.73	0.54
58:B1:78:LEU:O	58:B1:78:LEU:HD13	2.08	0.54
63:6:62:C:H5'	64:a:53:ARG:HE	1.73	0.54
65:0:105:VAL:O	65:0:337:ARG:NH1	2.41	0.54
15:O:53:ILE:HG12	53:3:1060:U:H5''	1.89	0.54
18:R:88:LEU:HD13	18:R:91:ARG:HD2	1.90	0.54
30:e:162:ASP:OD1	30:e:162:ASP:N	2.41	0.54
51:1:455:C:H3'	51:1:456:C:C5'	2.38	0.54
51:1:2572:A:H5'	51:1:2574:G:H4'	1.90	0.54
58:B1:30:ILE:HG21	58:B1:241:VAL:O	2.08	0.54
15:O:28:THR:HG21	15:O:90:LEU:HB3	1.90	0.53
51:1:886:A:N3	51:1:886:A:H2'	2.23	0.53
51:1:1558:C:H4'	51:1:1559:U:C5'	2.39	0.53
51:1:2029:G:O6	51:1:2032:G:H5''	2.08	0.53
53:3:346:G:H2'	53:3:347:G:O4'	2.08	0.53
53:3:1273:C:H2'	53:3:1274:A:O4'	2.07	0.53
59:B2:684:ASN:OD1	59:B2:687:ARG:NH2	2.41	0.53
59:B2:1117:LEU:HD12	59:B2:1195:ILE:HG12	1.90	0.53
13:M:95:MET:HE2	13:M:129:ALA:HB1	1.90	0.53
29:d:53:THR:HG21	51:1:452:G:C8	2.43	0.53
33:i:80:LYS:HD3	33:i:86:LYS:HD2	1.88	0.53
33:i:97:VAL:HG23	33:i:137:LEU:HD23	1.88	0.53
51:1:1028:A:N6	51:1:1125:G:H2'	2.24	0.53
53:3:1506:U:O2'	53:3:1507:A:H5'	2.09	0.53
58:B1:814:CYS:SG	58:B1:883:ARG:NH2	2.81	0.53
59:B2:811:ASN:HA	59:B2:815:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:a:163:TYR:HB2	64:a:171:ILE:HD12	1.89	0.53
51:1:161:A:C3'	51:1:162:U:H5''	2.36	0.53
53:3:1002:G:H2'	53:3:1003:G:O4'	2.07	0.53
58:B1:1155:ILE:HG13	58:B1:1210:ILE:HB	1.89	0.53
13:M:101:ALA:HB3	13:M:112:ASP:HB3	1.90	0.53
35:k:25:LEU:HD22	51:1:2562:U:H4'	1.89	0.53
37:m:46:ILE:O	37:m:103:TYR:OH	2.27	0.53
51:1:644:A:H2'	51:1:645:C:C5'	2.39	0.53
51:1:1018:U:O2'	51:1:1120:G:N2	2.41	0.53
53:3:166:U:H2'	53:3:167:A:C8	2.43	0.53
53:3:166:U:H2'	53:3:167:A:H8	1.74	0.53
58:B1:209:ASN:HA	58:B1:214:ARG:HH21	1.74	0.53
1:A:55:GLY:O	24:X:20:LYS:NZ	2.41	0.53
6:F:1:MET:HE3	51:1:2742:G:H5''	1.90	0.53
8:H:3:LYS:HA	53:3:1190:G:OP1	2.08	0.53
8:H:18:ASN:O	8:H:39:ARG:NH2	2.41	0.53
27:b:20:ASN:HB3	27:b:23:LEU:HD23	1.90	0.53
30:e:59:ILE:O	30:e:101:ARG:NH1	2.41	0.53
51:1:154:U:H2'	51:1:155:A:C8	2.44	0.53
51:1:186:G:H2'	51:1:187:G:H8	1.74	0.53
51:1:1172:C:H2'	51:1:1173:U:C6	2.43	0.53
51:1:2257:U:O2'	51:1:2258:C:H5'	2.09	0.53
53:3:231:U:H2'	53:3:232:G:C8	2.43	0.53
57:A1:16:ILE:HG23	57:A1:26:VAL:HG22	1.91	0.53
58:B1:746:LEU:HG	58:B1:758:PRO:HG3	1.90	0.53
9:I:59:LYS:NZ	9:I:193:ASP:OD2	2.42	0.53
28:c:24:VAL:HG21	28:c:188:LEU:HD23	1.91	0.53
28:c:77:ARG:NH2	28:c:200:ASP:OD2	2.40	0.53
31:f:103:ASN:ND2	31:f:113:ASP:OD1	2.41	0.53
51:1:575:A:O2'	51:1:576:U:H5'	2.08	0.53
51:1:1161:C:H2'	51:1:1162:G:H8	1.74	0.53
51:1:2106:U:H2'	51:1:2107:G:H4'	1.90	0.53
51:1:2760:C:O2'	51:1:2761:A:H5'	2.08	0.53
11:K:2:ARG:HH12	11:K:91:ARG:HB2	1.73	0.53
46:v:14:LYS:HB2	52:2:98:G:H1	1.74	0.53
51:1:1103:A:H3'	51:1:1104:C:H5''	1.91	0.53
51:1:1161:C:H2'	51:1:1162:G:C8	2.43	0.53
51:1:1611:C:H6	51:1:1611:C:H5'	1.72	0.53
51:1:1965:C:H5''	51:1:1966:A:H2'	1.89	0.53
51:1:2024:G:OP2	51:1:2034:U:H4'	2.09	0.53
53:3:112:G:N2	53:3:354:G:H5'	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1005:A:H2'	53:3:1006:G:H5'	1.90	0.53
53:3:1088:G:H21	53:3:1167:A:N6	2.03	0.53
57:A2:100:LEU:HD23	57:A2:115:ILE:HG21	1.89	0.53
58:B1:111:THR:HG22	58:B1:300:GLN:NE2	2.23	0.53
59:B2:628:HIS:HB3	59:B2:647:ARG:HH21	1.74	0.53
65:O:583:TYR:HB2	65:O:593:PHE:HZ	1.74	0.53
22:V:8:GLN:NE2	22:V:59:GLU:OE2	2.42	0.53
26:Z:38:GLU:HB2	53:3:1526:G:OP2	2.08	0.53
30:e:154:THR:HG21	51:1:2314:A:H1'	1.90	0.53
45:u:14:THR:OG1	45:u:68:ASN:ND2	2.41	0.53
46:v:35:GLU:OE2	46:v:93:ARG:NH1	2.42	0.53
48:x:17:ARG:CG	51:1:380:G:H5'	2.36	0.53
51:1:455:C:H3'	51:1:456:C:H5''	1.91	0.53
51:1:1123:C:H2'	51:1:1124:G:H8	1.73	0.53
51:1:1141:U:H4'	51:1:1142:A:O4'	2.09	0.53
51:1:1726:C:H2'	51:1:1727:C:C6	2.44	0.53
51:1:2720:U:H6	51:1:2720:U:H5'	1.73	0.53
53:3:1042:A:H2'	53:3:1043:G:O4'	2.09	0.53
53:3:1176:A:H2'	53:3:1177:G:C8	2.44	0.53
57:A1:100:LEU:HD21	57:A1:121:VAL:HG11	1.90	0.53
58:B1:68:TYR:CA	58:B1:75:TYR:HE2	2.22	0.53
58:B1:975:ILE:HD11	58:B1:1003:LEU:HD11	1.91	0.53
26:Z:25:ALA:HA	26:Z:28:LEU:HB2	1.90	0.53
28:c:56:LYS:CE	51:1:2830:C:H5''	2.39	0.53
29:d:119:ILE:HB	29:d:187:VAL:HG12	1.91	0.53
38:n:49:GLU:HB3	51:1:2839:G:H4'	1.91	0.53
51:1:940:G:H2'	51:1:941:A:C5'	2.39	0.53
53:3:410:G:H2'	53:3:429:U:C5	2.44	0.53
53:3:1436:U:H2'	53:3:1437:A:C8	2.43	0.53
59:B2:243:PRO:HB2	59:B2:274:ILE:HG23	1.90	0.53
1:A:62:LYS:HG3	24:X:20:LYS:HB3	1.91	0.53
11:K:5:GLU:HB2	11:K:90:MET:HB2	1.90	0.53
12:L:78:ARG:C	12:L:80:GLY:H	2.17	0.53
15:O:67:ILE:HG23	19:S:95:LEU:HD23	1.91	0.53
45:u:86:PHE:HE1	45:u:91:LYS:HG3	1.74	0.53
51:1:1345:C:H6	51:1:1345:C:H5'	1.74	0.53
51:1:2869:G:H2'	51:1:2870:C:O4'	2.09	0.53
53:3:3:A:H5'	53:3:613:C:H4'	1.91	0.53
53:3:608:A:H2'	53:3:609:A:O4'	2.08	0.53
53:3:1014:A:H2	53:3:1219:A:H1'	1.73	0.53
13:M:42:GLU:HG2	13:M:100:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:75:GLN:HB2	13:M:127:TYR:HB2	1.90	0.52
44:t:31:VAL:HG12	44:t:84:TYR:HA	1.91	0.52
49:y:21:LEU:HA	49:y:25:GLN:HB3	1.91	0.52
51:1:917:A:H2	52:2:79:G:N3	2.07	0.52
51:1:1273:U:H4'	51:1:1275:A:OP1	2.08	0.52
59:B2:246:LEU:HB3	59:B2:269:ILE:HD13	1.91	0.52
65:0:388:LEU:HD23	65:0:391:VAL:HG11	1.91	0.52
29:d:68:ALA:HA	51:1:1255:U:C5	2.44	0.52
36:l:47:ARG:NH2	51:1:251:A:H4'	2.25	0.52
51:1:154:U:H2'	51:1:155:A:H8	1.74	0.52
51:1:817:C:O2'	51:1:839:U:H5''	2.10	0.52
53:3:1391:U:H2'	53:3:1392:G:C8	2.44	0.52
58:B1:39:LYS:O	58:B1:273:ILE:HG23	2.08	0.52
13:M:29:SER:HB3	53:3:589:U:H5''	1.90	0.52
30:e:65:LEU:HD22	52:2:42:C:C4	2.44	0.52
51:1:2625:G:H2'	51:1:2626:C:O4'	2.09	0.52
53:3:134:G:H2'	53:3:135:C:O4'	2.08	0.52
53:3:235:C:H2'	53:3:236:A:C8	2.44	0.52
53:3:1054:C:H4'	53:3:1056:U:OP2	2.09	0.52
53:3:1270:G:H2'	53:3:1271:A:H8	1.75	0.52
11:K:36:ILE:HG22	11:K:64:VAL:HG13	1.92	0.52
22:V:11:VAL:HG13	22:V:20:ILE:HD11	1.90	0.52
39:o:10:ARG:HD2	51:1:2294:G:OP1	2.10	0.52
57:A1:47:LEU:HD23	57:A1:51:MET:HG3	1.89	0.52
58:B1:111:THR:HG23	58:B1:300:GLN:NE2	2.24	0.52
58:B1:112:ALA:HA	58:B1:238:ILE:HA	1.91	0.52
65:0:53:MET:HE1	65:0:472:ARG:HG3	1.91	0.52
12:L:91:ARG:NE	12:L:91:ARG:HA	2.25	0.52
34:j:118:MET:HA	34:j:121:LYS:HD3	1.91	0.52
51:1:2628:C:H3'	51:1:2629:U:H5'	1.92	0.52
58:B1:201:LEU:HD12	58:B1:224:LEU:HD12	1.92	0.52
58:B1:205:LEU:HG	58:B1:217:LEU:HB3	1.90	0.52
59:B2:714:VAL:HB	59:B2:787:PRO:HD2	1.92	0.52
51:1:1066:U:H2'	51:1:1068:G:OP2	2.08	0.52
51:1:2818:U:H2'	51:1:2819:G:H8	1.75	0.52
17:Q:4:ASN:HB3	22:V:35:LYS:HE2	1.91	0.52
36:l:81:ASP:OD1	36:l:81:ASP:N	2.38	0.52
40:p:84:SER:OG	40:p:86:LYS:NZ	2.42	0.52
51:1:857:G:H2'	51:1:858:G:O4'	2.10	0.52
51:1:1869:G:H3'	51:1:1870:C:H5'	1.92	0.52
51:1:2800:A:C2	51:1:2895:G:H1'	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:B2:125:GLY:HA2	59:B2:499:SER:HB2	1.92	0.52
59:B2:524:ILE:HG21	59:B2:708:VAL:HG13	1.92	0.52
30:e:65:LEU:CD1	52:2:41:G:H2'	2.40	0.52
51:1:685:A:H5''	51:1:788:A:H62	1.74	0.52
53:3:604:G:H2'	53:3:605:U:O4'	2.10	0.52
53:3:1278:G:OP1	53:3:1279:G:H5'	2.10	0.52
53:3:1353:G:O2'	53:3:1354:U:H5'	2.10	0.52
53:3:1450:U:H1'	53:3:1454:G:N2	2.25	0.52
65:0:91:GLY:N	69:0:802:PO4:O1	2.40	0.52
65:0:282:VAL:HA	65:0:286:LEU:HD12	1.91	0.52
9:I:53:GLN:HA	9:I:198:LEU:HD12	1.92	0.52
10:J:76:ASN:HB2	10:J:81:GLN:HG2	1.92	0.52
16:P:19:VAL:HG22	16:P:82:GLU:HB2	1.92	0.52
23:W:33:THR:OG1	23:W:34:GLU:N	2.43	0.52
39:o:51:ALA:HB3	39:o:78:VAL:HG12	1.92	0.52
51:1:686:U:H3'	51:1:687:C:H5'	1.91	0.52
51:1:973:A:H5'	51:1:1188:U:H1'	1.92	0.52
51:1:1672:A:C2	51:1:2582:G:H5'	2.44	0.52
53:3:1247:U:O2'	53:3:1248:A:H5'	2.10	0.52
57:A2:43:LEU:HD13	57:A2:217:ILE:HD11	1.90	0.52
58:B1:412:LEU:HD23	58:B1:416:ILE:HG13	1.92	0.52
58:B1:832:LYS:HB3	58:B1:1242:ARG:NH1	2.24	0.52
20:T:57:ARG:NH2	20:T:58:MET:SD	2.82	0.52
27:b:140:VAL:HA	27:b:191:LEU:HA	1.92	0.52
51:1:118:A:OP2	51:1:119:A:H5''	2.10	0.52
51:1:528:A:H2'	51:1:529:A:H5''	1.91	0.52
51:1:937:C:H2'	51:1:938:G:H8	1.74	0.52
51:1:2114:A:C5	51:1:2115:G:H1'	2.45	0.52
53:3:86:G:H4'	53:3:87:C:C5	2.45	0.52
53:3:123:U:OP1	53:3:312:C:H5'	2.10	0.52
4:D:8:SER:HA	51:1:1309:G:H5''	1.91	0.51
25:Y:22:SER:HA	53:3:1458:G:O3'	2.11	0.51
33:i:69:VAL:O	33:i:71:LYS:NZ	2.43	0.51
51:1:519:U:H2'	51:1:520:G:C8	2.45	0.51
51:1:1064:C:H2'	51:1:1065:U:C6	2.44	0.51
51:1:1138:G:H2'	51:1:1139:G:O4'	2.10	0.51
51:1:2650:U:H2'	51:1:2651:C:H6	1.74	0.51
53:3:473:U:H2'	53:3:474:G:C8	2.45	0.51
53:3:779:C:H2'	53:3:780:A:O4'	2.10	0.51
53:3:1402:C:H2'	53:3:1403:C:O4'	2.10	0.51
57:A1:205:MET:HE3	57:A1:213:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:290:ILE:HG21	61:NG:93:ILE:O	2.09	0.51
58:B1:375:GLU:HG2	59:B2:1245:ALA:O	2.10	0.51
8:H:78:LYS:HB3	59:B2:947:GLU:OE2	2.11	0.51
41:q:54:ARG:NH2	51:1:1155:A:H4'	2.25	0.51
48:x:7:THR:HG23	48:x:9:LYS:HG3	1.92	0.51
48:x:18:SER:HB2	51:1:2080:A:H5'	1.91	0.51
51:1:749:A:C2	51:1:1618:A:H2'	2.45	0.51
51:1:2432:A:H5'	63:6:76:A:O3'	2.09	0.51
53:3:210:C:H5'	53:3:211:G:N3	2.25	0.51
53:3:1042:A:H2'	53:3:1043:G:C1'	2.40	0.51
53:3:1412:C:H2'	53:3:1413:A:C8	2.45	0.51
57:A2:140:ILE:HD12	57:A2:142:MET:HE3	1.91	0.51
58:B1:144:TYR:CE1	58:B1:162:GLU:CD	2.88	0.51
8:H:13:ILE:HG13	8:H:14:VAL:HG23	1.91	0.51
29:d:58:LYS:NZ	29:d:62:GLN:OE1	2.43	0.51
32:g:84:ALA:HB2	32:g:148:ALA:HB1	1.90	0.51
36:l:108:ALA:HB3	36:l:125:LEU:HD11	1.92	0.51
51:1:1447:C:H2'	51:1:1448:G:H8	1.75	0.51
51:1:1637:A:H5'	51:1:1760:C:O2'	2.10	0.51
53:3:1449:C:H2'	53:3:1450:U:O4'	2.10	0.51
53:3:1481:U:O2'	53:3:1482:G:H5'	2.09	0.51
58:B1:850:LYS:HB2	58:B1:857:LEU:HB2	1.91	0.51
9:I:205:LYS:HE3	53:3:8:A:C5	2.45	0.51
11:K:40:GLU:OE2	11:K:100:SER:OG	2.28	0.51
17:Q:45:ASN:HB3	53:3:528:C:H41	1.75	0.51
27:b:106:PRO:HA	27:b:194:VAL:HA	1.92	0.51
39:o:21:LEU:HD11	51:1:2379:G:H4'	1.91	0.51
51:1:1068:G:O2'	51:1:1096:A:H4'	2.10	0.51
53:3:757:U:H2'	53:3:758:C:O4'	2.10	0.51
53:3:1411:C:H2'	53:3:1412:C:C6	2.45	0.51
58:B1:505:ASP:OD2	59:B2:812:PHE:HA	2.11	0.51
2:B:37:HIS:ND1	2:B:38:LEU:O	2.41	0.51
11:K:38:ARG:NH1	11:K:40:GLU:OE1	2.43	0.51
41:q:82:LEU:HD23	41:q:112:ALA:HB2	1.92	0.51
51:1:1625:C:H2'	51:1:1626:A:O4'	2.11	0.51
51:1:1906:G:H2'	51:1:1907:G:H5''	1.93	0.51
59:B2:786:GLY:N	59:B2:789:THR:OG1	2.41	0.51
65:0:105:VAL:HG22	65:0:337:ARG:HH11	1.75	0.51
65:0:116:VAL:HG11	65:0:146:ARG:HD3	1.91	0.51
65:0:503:GLY:N	65:0:518:VAL:O	2.40	0.51
7:G:103:TRP:HA	7:G:106:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:2:LYS:HG2	53:3:1048:G:H5''	1.92	0.51
23:W:41:SER:HB3	23:W:51:GLN:HE21	1.76	0.51
27:b:106:PRO:HD2	27:b:109:LEU:HD13	1.91	0.51
29:d:63:LYS:HD3	51:1:2443:C:OP1	2.10	0.51
29:d:145:ASP:HA	29:d:166:LYS:HB3	1.91	0.51
31:f:40:VAL:O	31:f:54:ARG:NH2	2.43	0.51
51:1:1669:A:O3'	51:1:2549:G:H5'	2.11	0.51
58:B1:633:ALA:HB2	59:B2:808:ASN:N	2.19	0.51
65:0:97:ILE:HD11	65:0:443:PRO:HD2	1.93	0.51
65:0:151:PHE:HE2	65:0:171:LEU:HG	1.75	0.51
9:I:82:LYS:O	9:I:88:ASN:ND2	2.36	0.51
27:b:257:ARG:HH12	51:1:1799:G:H3'	1.76	0.51
51:1:368:A:O2'	51:1:369:U:H5'	2.11	0.51
51:1:558:U:H2'	51:1:559:G:H8	1.75	0.51
51:1:644:A:H2'	51:1:645:C:C4'	2.41	0.51
53:3:701:U:C4'	53:3:703:G:H1'	2.41	0.51
58:B1:99:ARG:HA	58:B1:248:ASP:HB2	1.92	0.51
65:0:170:GLN:HE21	65:0:266:CYS:H	1.59	0.51
51:1:1542:U:H2'	51:1:1543:G:O4'	2.10	0.51
51:1:2165:C:H5''	51:1:2166:U:OP1	2.10	0.51
53:3:406:G:O2'	53:3:407:U:H5'	2.11	0.51
53:3:1138:G:H3'	53:3:1138:G:N3	2.25	0.51
58:B1:215:LYS:HA	58:B1:218:THR:HG22	1.92	0.51
58:B1:390:LEU:N	58:B1:390:LEU:CD1	2.73	0.51
20:T:13:GLU:O	20:T:83:ARG:NH2	2.42	0.51
23:W:70:THR:OG1	23:W:71:ASP:N	2.44	0.51
30:e:31:GLU:HB2	30:e:156:THR:HB	1.93	0.51
51:1:1907:G:H2'	51:1:1908:C:O4'	2.10	0.51
53:3:184:G:H4'	53:3:224:U:O3'	2.11	0.51
53:3:392:C:H2'	53:3:393:A:H8	1.76	0.51
58:B1:99:ARG:HG3	58:B1:99:ARG:HH11	1.74	0.51
58:B1:437:PHE:HZ	58:B1:453:VAL:HG11	1.76	0.51
65:0:158:ILE:HB	65:0:166:PRO:HG3	1.92	0.51
9:I:73:ASN:OD1	9:I:76:LYS:NZ	2.44	0.51
32:g:78:VAL:HG11	32:g:103:VAL:HG22	1.91	0.51
33:i:11:GLN:HB2	33:i:56:VAL:HG12	1.93	0.51
46:v:66:ASP:O	46:v:68:LYS:NZ	2.43	0.51
51:1:543:G:H3'	51:1:544:C:H5''	1.93	0.51
51:1:878:A:H3'	51:1:879:G:H8	1.76	0.51
51:1:2186:G:H2'	51:1:2187:U:O4'	2.11	0.51
53:3:267:C:O2	53:3:267:C:H2'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1206:G:H2'	53:3:1207:G:O4'	2.11	0.51
58:B1:289:ASP:H	61:NG:104:SER:CB	2.23	0.51
58:B1:749:LYS:HB3	58:B1:755:ILE:HD11	1.93	0.51
59:B2:93:SER:HA	59:B2:128:PRO:HA	1.93	0.51
65:0:158:ILE:HG23	65:0:162:LEU:HD12	1.92	0.51
22:V:44:HIS:HB3	22:V:70:LYS:HG3	1.92	0.50
33:i:91:LYS:HB2	33:i:94:LYS:HB2	1.92	0.50
42:r:10:LYS:HE2	51:1:994:C:O2'	2.11	0.50
53:3:1137:C:H4'	53:3:1138:G:C2	2.45	0.50
65:0:342:VAL:HG12	65:0:378:ARG:HA	1.91	0.50
1:A:54:GLY:H	24:X:26:ASP:HA	1.76	0.50
4:D:24:THR:O	4:D:28:ARG:NH1	2.44	0.50
51:1:226:A:H2'	51:1:227:A:O4'	2.11	0.50
51:1:1019:U:OP1	51:1:1035:U:O2'	2.29	0.50
51:1:2404:U:H2'	51:1:2405:G:O4'	2.10	0.50
51:1:2586:U:H2'	51:1:2587:A:C8	2.46	0.50
52:2:118:C:H2'	52:2:119:A:C4'	2.40	0.50
53:3:1421:G:C5	53:3:1422:G:H1'	2.45	0.50
59:B2:255:ILE:HB	59:B2:263:VAL:HB	1.92	0.50
16:P:121:ARG:HH22	53:3:1524:C:H5''	1.75	0.50
47:w:70:PRO:HD3	52:2:12:C:N4	2.26	0.50
51:1:2104:C:H2'	51:1:2105:U:O4'	2.11	0.50
51:1:2743:U:C2'	51:1:2744:G:H5''	2.40	0.50
51:1:2881:U:H2'	51:1:2882:A:C8	2.46	0.50
53:3:407:U:H2'	53:3:408:A:C8	2.45	0.50
65:0:312:SER:OG	65:0:313:ASP:N	2.45	0.50
5:E:2:LYS:HG3	51:1:242:G:C8	2.47	0.50
37:m:1:MET:HE1	62:5:63:G:O2'	2.11	0.50
51:1:663:G:C3'	51:1:664:G:H5''	2.41	0.50
51:1:2041:U:H2'	51:1:2042:A:C8	2.47	0.50
51:1:2250:G:H21	51:1:2496:C:H5''	1.76	0.50
51:1:2663:G:H8	51:1:2663:G:OP2	1.94	0.50
53:3:839:C:H2'	53:3:840:C:C6	2.46	0.50
58:B1:421:VAL:O	58:B1:436:ALA:HA	2.12	0.50
62:5:23:A:H2'	62:5:24:G:C8	2.47	0.50
64:a:12:ARG:HA	64:a:15:VAL:HB	1.92	0.50
13:M:104:SER:O	53:3:642:A:H2	1.93	0.50
14:N:27:ILE:HD12	14:N:34:LEU:HD22	1.93	0.50
34:j:2:LYS:HA	51:1:995:C:N3	2.27	0.50
53:3:14:U:O2	53:3:17:U:H5	1.95	0.50
53:3:91:U:H2'	53:3:92:U:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:195:A:H2'	53:3:196:A:C8	2.47	0.50
58:B1:972:LYS:HD2	58:B1:1004:ALA:HA	1.93	0.50
59:B2:974:ARG:HD2	59:B2:1014:LEU:HD21	1.92	0.50
65:0:139:ALA:N	65:0:263:LEU:O	2.43	0.50
4:D:10:LEU:HD23	51:1:770:G:H5''	1.94	0.50
33:i:92:PRO:HD2	51:1:1076:C:O2'	2.12	0.50
51:1:473:G:O2'	51:1:474:G:H5'	2.12	0.50
51:1:1159:U:H2'	51:1:1160:G:C8	2.46	0.50
51:1:1536:C:H4'	51:1:1537:G:N2	2.27	0.50
51:1:1999:C:H5''	51:1:2723:C:O2'	2.12	0.50
51:1:2041:U:H2'	51:1:2042:A:H8	1.77	0.50
51:1:2266:A:H4'	51:1:2267:A:N3	2.26	0.50
51:1:2742:G:H1	51:1:2762:C:H42	1.60	0.50
53:3:35:G:H2'	53:3:36:C:C6	2.46	0.50
59:B2:9:LYS:HG2	59:B2:1171:ARG:HH12	1.77	0.50
59:B2:400:VAL:HG21	59:B2:452:ARG:HE	1.76	0.50
62:5:22:G:H2'	62:5:23:A:C8	2.47	0.50
29:d:45:ALA:HB2	29:d:89:PRO:HD3	1.93	0.50
33:i:8:VAL:HG11	33:i:26:ALA:HB1	1.93	0.50
33:i:14:ALA:HB1	33:i:45:THR:HG23	1.94	0.50
33:i:53:PRO:HD2	33:i:77:VAL:HB	1.94	0.50
43:s:75:PHE:HE1	51:1:519:U:H1'	1.77	0.50
51:1:140:C:H2'	51:1:141:G:H4'	1.94	0.50
51:1:161:A:H3'	51:1:162:U:C5'	2.39	0.50
53:3:1109:C:H2'	53:3:1110:A:O4'	2.12	0.50
53:3:1441:A:H62	53:3:1461:G:H21	1.60	0.50
65:0:105:VAL:HG22	65:0:337:ARG:HD3	1.94	0.50
65:0:364:VAL:HG12	65:0:366:MET:H	1.77	0.50
8:H:22:PHE:HE2	15:O:11:LYS:HD3	1.76	0.50
11:K:62:MET:HB3	11:K:64:VAL:HG23	1.93	0.50
51:1:948:C:H2'	51:1:949:G:H8	1.77	0.50
53:3:89:U:H2'	53:3:90:C:O4'	2.12	0.50
65:0:420:VAL:HG21	65:0:481:ALA:HB1	1.93	0.50
9:I:104:MET:HG3	9:I:172:VAL:HG22	1.92	0.50
16:P:127:ARG:HB2	53:3:796:C:OP1	2.12	0.50
27:b:59:GLN:HG2	27:b:84:PRO:HB2	1.93	0.50
34:j:45:THR:HB	34:j:48:VAL:HG22	1.93	0.50
51:1:748:G:O2'	51:1:749:A:H5''	2.11	0.50
51:1:1443:U:H2'	51:1:1444:G:H8	1.75	0.50
53:3:76:G:H2'	53:3:77:A:C5'	2.42	0.50
53:3:458:U:H2'	53:3:459:A:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1386:G:H2'	53:3:1387:G:H8	1.77	0.50
66:h:6:5OH:N	66:h:6:5OH:CS	2.75	0.50
59:B2:554:HIS:HD2	59:B2:558:VAL:HB	1.77	0.49
65:0:94:ASP:HB3	65:0:465:HIS:HB2	1.93	0.49
10:J:37:VAL:HG11	10:J:113:VAL:HA	1.95	0.49
24:X:17:LYS:O	24:X:20:LYS:NZ	2.41	0.49
51:1:859:G:HO2'	51:1:860:U:H6	1.59	0.49
51:1:1472:C:H2'	51:1:1473:G:C8	2.47	0.49
51:1:1645:G:H5''	51:1:1646:C:C5'	2.27	0.49
53:3:253:A:H2'	53:3:254:G:C8	2.47	0.49
53:3:781:A:OP1	53:3:1523:G:H5'	2.13	0.49
53:3:1023:U:H2'	53:3:1024:G:C8	2.47	0.49
59:B2:18:ARG:HE	59:B2:620:ASN:HA	1.77	0.49
59:B2:232:ILE:HG12	59:B2:237:LEU:HG	1.93	0.49
7:G:100:LEU:HB2	7:G:174:GLU:HG2	1.93	0.49
21:U:4:ILE:HG12	21:U:21:VAL:HG22	1.94	0.49
26:Z:32:ARG:HG3	26:Z:33:ARG:HG2	1.94	0.49
31:f:28:LYS:N	31:f:78:VAL:O	2.46	0.49
46:v:45:ASP:N	46:v:45:ASP:OD1	2.44	0.49
48:x:5:GLN:O	48:x:73:ARG:NH2	2.45	0.49
51:1:355:U:H2'	51:1:356:G:C8	2.47	0.49
51:1:864:G:H4'	52:2:101:A:H4'	1.94	0.49
53:3:359:G:H2'	53:3:360:G:O4'	2.13	0.49
53:3:599:C:H2'	53:3:600:A:C8	2.47	0.49
53:3:1316:G:C2'	53:3:1317:C:H5''	2.40	0.49
58:B1:102:MET:HG2	58:B1:246:PRO:HD3	1.94	0.49
58:B1:275:ARG:HH12	58:B1:278:ARG:NH1	2.09	0.49
59:B2:400:VAL:HG11	59:B2:452:ARG:HD2	1.94	0.49
59:B2:1070:HIS:NE2	59:B2:1114:GLU:OE1	2.36	0.49
62:5:51:U:H2'	62:5:52:G:C8	2.48	0.49
27:b:201:LEU:CD2	53:3:773:G:H5''	2.42	0.49
37:m:17:ASN:ND2	37:m:97:GLN:OE1	2.36	0.49
51:1:274:C:H2'	51:1:275:C:O4'	2.12	0.49
51:1:341:C:H2'	51:1:342:A:C8	2.47	0.49
51:1:1434:A:H2'	51:1:1435:G:H8	1.77	0.49
51:1:2208:C:H2'	51:1:2209:G:C8	2.47	0.49
51:1:2811:G:H2'	51:1:2812:G:H8	1.77	0.49
53:3:38:G:H22	53:3:397:A:H5'	1.77	0.49
53:3:1013:G:N2	53:3:1015:G:H3'	2.27	0.49
60:W0:3:ARG:NH1	60:W0:55:GLU:OE2	2.40	0.49
64:a:166:ASP:OD2	64:a:172:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:129:PHE:HA	8:H:132:ALA:HB3	1.93	0.49
12:L:110:ARG:NH1	12:L:125:ASP:OD2	2.46	0.49
15:O:65:TYR:HB3	19:S:95:LEU:HD22	1.95	0.49
32:g:7:ASP:HA	32:g:15:LEU:HD23	1.94	0.49
33:i:92:PRO:HB2	51:1:1077:A:C4'	2.41	0.49
33:i:92:PRO:HB3	51:1:1077:A:H1'	1.92	0.49
38:n:22:ARG:HG3	38:n:70:THR:HA	1.93	0.49
51:1:1326:U:H2'	51:1:1327:A:C8	2.41	0.49
51:1:1735:A:H2'	51:1:1736:U:O4'	2.11	0.49
51:1:2469:A:H2'	51:1:2470:G:O4'	2.12	0.49
2:B:27:LEU:HD13	2:B:36:LYS:HB3	1.95	0.49
9:I:50:TYR:CD2	53:3:508:U:H4'	2.48	0.49
21:U:14:ARG:NH1	53:3:618:C:H1'	2.21	0.49
28:c:4:LEU:HD23	28:c:29:VAL:HG11	1.94	0.49
38:n:49:GLU:CB	51:1:2839:G:H4'	2.42	0.49
47:w:12:SER:HB3	51:1:2261:C:C6	2.47	0.49
51:1:2104:C:H42	51:1:2185:U:H3	1.60	0.49
53:3:422:C:H4'	53:3:423:G:C4	2.48	0.49
53:3:1391:U:H2'	53:3:1392:G:H8	1.77	0.49
53:3:1492:A:H1'	54:4:5:U:O2'	2.13	0.49
58:B1:550:VAL:O	58:B1:569:LEU:HA	2.13	0.49
58:B1:683:ILE:HD12	58:B1:754:ILE:HG21	1.93	0.49
25:Y:54:GLN:HE21	53:3:193:C:C1'	2.25	0.49
29:d:94:GLN:CD	51:1:660:C:H5''	2.38	0.49
43:s:18:ARG:NH1	51:1:518:G:H4'	2.28	0.49
51:1:1029:A:H2'	51:1:1030:C:O4'	2.13	0.49
51:1:1417:C:C4'	51:1:1587:G:H21	2.26	0.49
53:3:70:U:H4'	53:3:71:A:H8	1.78	0.49
58:B1:1179:PRO:HD2	58:B1:1184:ASP:HA	1.93	0.49
11:K:49:TYR:OH	23:W:62:ARG:O	2.30	0.49
14:N:121:ARG:HD2	53:3:1348:U:H4'	1.95	0.49
40:p:61:ARG:NH2	40:p:99:LEU:O	2.44	0.49
51:1:934:U:H2'	51:1:935:C:C6	2.47	0.49
51:1:948:C:H2'	51:1:949:G:C8	2.47	0.49
51:1:1597:A:H5''	51:1:1598:A:H5'	1.94	0.49
51:1:2364:C:H2'	51:1:2365:G:O4'	2.13	0.49
51:1:2792:A:C3'	51:1:2793:C:H5''	2.43	0.49
53:3:952:U:H2'	53:3:953:G:H8	1.78	0.49
53:3:1128:C:O2'	53:3:1129:C:H5'	2.13	0.49
55:8:3:DC:H2''	55:8:4:DT:C7	2.42	0.49
57:A1:100:LEU:HB2	57:A1:144:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:B2:565:GLU:HA	59:B2:569:ILE:HG12	1.95	0.49
65:0:433:LEU:O	65:0:437:ARG:N	2.45	0.49
21:U:70:ARG:NH2	53:3:451:A:OP2	2.45	0.49
24:X:54:ARG:HG3	24:X:55:GLN:HG2	1.95	0.49
28:c:45:TYR:CZ	51:1:2637:U:H5'	2.47	0.49
31:f:48:THR:OG1	31:f:49:LEU:N	2.45	0.49
44:t:64:LYS:HE2	51:1:1601:G:OP1	2.13	0.49
51:1:26:G:H1'	51:1:515:A:H61	1.77	0.49
51:1:1111:A:H2'	51:1:1111:A:N3	2.28	0.49
53:3:17:U:H2'	53:3:18:C:C6	2.48	0.49
53:3:916:U:H2'	53:3:917:G:C8	2.47	0.49
58:B1:201:LEU:HD11	58:B1:220:ARG:HG2	1.95	0.49
58:B1:1371:ARG:HE	58:B1:1372:ARG:NH1	2.10	0.49
65:0:289:PRO:HB3	65:0:337:ARG:HH21	1.78	0.49
21:U:56:ARG:HA	21:U:59:HIS:HB3	1.95	0.49
51:1:1020:A:C1'	51:1:1021:A:OP2	2.60	0.49
53:3:745:G:OP1	53:3:852:G:H5'	2.13	0.49
53:3:1491:G:H2'	66:h:6:5OH:O	2.13	0.49
58:B1:115:TRP:O	58:B1:1333:THR:HG21	2.13	0.49
58:B1:145:VAL:HG12	58:B1:184:ALA:HB1	1.94	0.49
59:B2:533:LEU:HD13	59:B2:540:ARG:HH21	1.77	0.49
7:G:53:LEU:HD22	7:G:219:THR:HG21	1.95	0.48
17:Q:71:HIS:HB2	17:Q:73:LEU:HD23	1.95	0.48
30:e:36:ASN:HB3	30:e:152:ASP:HB3	1.95	0.48
42:r:9:GLY:O	51:1:996:A:H1'	2.13	0.48
43:s:4:ILE:HG22	43:s:106:VAL:HG13	1.93	0.48
51:1:2220:U:H2'	51:1:2221:G:C8	2.47	0.48
52:2:28:C:H2'	52:2:29:A:C8	2.48	0.48
53:3:632:U:H3'	53:3:633:G:H5'	1.94	0.48
53:3:802:A:H2'	53:3:803:G:O4'	2.13	0.48
57:A1:18:GLN:HA	57:A1:24:ALA:HA	1.94	0.48
63:6:44:A:H3'	63:6:45:G:H5''	1.96	0.48
16:P:27:ASN:ND2	53:3:692:U:H5	2.11	0.48
50:z:40:THR:HG22	50:z:43:ILE:HG12	1.94	0.48
51:1:1180:U:H5''	51:1:1181:U:H5	1.78	0.48
53:3:530:G:H3'	53:3:531:U:H5'	1.95	0.48
57:A1:182:ARG:O	57:A1:205:MET:HA	2.13	0.48
58:B1:220:ARG:HG2	58:B1:220:ARG:NH1	2.26	0.48
63:6:68:C:H2'	63:6:69:C:C6	2.48	0.48
65:0:127:TRP:O	65:0:131:ASN:ND2	2.45	0.48
8:H:80:GLY:O	8:H:84:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:96:ASN:N	12:L:96:ASN:OD1	2.46	0.48
51:1:616:A:H2'	51:1:617:G:O4'	2.12	0.48
51:1:686:U:H6	51:1:788:A:N1	2.12	0.48
51:1:1474:U:H2'	51:1:1475:G:H5'	1.96	0.48
51:1:1753:G:H22	51:1:1755:A:H3'	1.79	0.48
51:1:2128:G:H1	51:1:2160:C:H42	1.58	0.48
51:1:2176:A:H5'	64:a:219:GLY:C	2.38	0.48
51:1:2522:U:H2'	51:1:2523:G:H5'	1.96	0.48
53:3:141:G:H2'	53:3:142:G:O4'	2.13	0.48
53:3:681:A:H2'	53:3:682:G:C8	2.48	0.48
53:3:701:U:H4'	53:3:703:G:H1'	1.93	0.48
56:9:27:DC:OP2	59:B2:542:ARG:CZ	2.61	0.48
58:B1:770:LEU:CD1	59:B2:618:GLN:HG3	2.37	0.48
63:6:37:A:H2'	63:6:38:A:O4'	2.13	0.48
28:c:79:LEU:HD12	51:1:2635:A:H4'	1.96	0.48
29:d:125:SER:O	29:d:137:LYS:NZ	2.39	0.48
30:e:115:GLY:HA3	30:e:177:ARG:HA	1.95	0.48
30:e:128:SER:HB2	30:e:154:THR:HG23	1.95	0.48
33:i:92:PRO:CG	51:1:1077:A:H1'	2.43	0.48
41:q:111:LYS:HD2	42:r:48:LYS:HD3	1.95	0.48
51:1:1335:C:H2'	51:1:1336:A:C8	2.48	0.48
51:1:2122:U:H2'	51:1:2123:G:H4'	1.95	0.48
59:B2:411:ARG:NH2	59:B2:427:ASP:OD2	2.44	0.48
59:B2:862:LEU:H	59:B2:862:LEU:HD13	1.77	0.48
64:a:46:VAL:HG13	64:a:212:VAL:HG22	1.94	0.48
65:0:12:ASN:HA	65:0:85:ASN:HB2	1.94	0.48
7:G:165:ALA:HB1	7:G:172:ILE:HD13	1.96	0.48
9:I:73:ASN:HA	9:I:76:LYS:HD2	1.95	0.48
17:Q:33:CYS:H	17:Q:54:VAL:HG13	1.78	0.48
47:w:20:LYS:HE3	51:1:2355:G:O2'	2.13	0.48
51:1:248:G:O5'	51:1:249:C:H5''	2.14	0.48
51:1:435:C:H2'	51:1:436:C:H5'	1.95	0.48
51:1:1357:C:H2'	51:1:1358:G:O4'	2.14	0.48
51:1:1447:C:H2'	51:1:1448:G:C8	2.48	0.48
51:1:2565:A:O2'	51:1:2566:A:H5'	2.13	0.48
51:1:2583:G:H2'	51:1:2584:U:O4'	2.13	0.48
52:2:32:U:H2'	52:2:33:G:O4'	2.14	0.48
52:2:101:A:H2'	52:2:102:G:O4'	2.13	0.48
53:3:207:C:C2'	53:3:208:U:H5''	2.43	0.48
53:3:591:U:H2'	53:3:592:G:C8	2.48	0.48
53:3:1220:G:H2'	53:3:1221:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8:22:DC:C4	58:B1:255:LEU:HD22	2.49	0.48
58:B1:1361:THR:OG1	59:B2:1282:GLY:O	2.28	0.48
59:B2:318:SER:OG	59:B2:320:ASP:OD1	2.31	0.48
8:H:152:VAL:HG12	8:H:197:VAL:HG13	1.96	0.48
15:O:7:ARG:HA	15:O:75:ASP:HA	1.96	0.48
38:n:32:GLU:HG2	38:n:115:LEU:HD12	1.94	0.48
40:p:61:ARG:HH21	40:p:99:LEU:HB3	1.79	0.48
51:1:2165:C:H41	51:1:2171:A:H61	1.60	0.48
51:1:2366:A:H2'	51:1:2367:G:O4'	2.13	0.48
51:1:2644:G:O2'	51:1:2645:G:H5'	2.13	0.48
53:3:591:U:H2'	53:3:592:G:H8	1.78	0.48
54:4:44:G:OP1	59:B2:1073:LYS:NZ	2.37	0.48
55:8:14:DC:H2'	55:8:15:DC:H6	1.79	0.48
58:B1:103:GLY:H	58:B1:244:VAL:HG22	1.79	0.48
58:B1:255:LEU:HD23	58:B1:261:ALA:HB2	1.95	0.48
18:R:99:GLN:HB3	53:3:949:A:OP1	2.13	0.48
39:o:104:GLN:NE2	39:o:108:ASP:OD2	2.47	0.48
40:p:1:SER:N	51:1:2875:C:H4'	2.27	0.48
46:v:14:LYS:HB2	52:2:98:G:N1	2.28	0.48
51:1:704:G:H1'	51:1:726:G:N2	2.28	0.48
51:1:1701:A:C2'	51:1:1702:G:H5'	2.43	0.48
51:1:2898:U:H2'	51:1:2899:A:H8	1.78	0.48
53:3:59:A:N6	53:3:331:G:H1'	2.28	0.48
55:8:14:DC:H2'	55:8:15:DC:C6	2.48	0.48
58:B1:809:VAL:HG21	58:B1:909:ILE:HG12	1.95	0.48
59:B2:1314:GLN:HB2	60:W0:28:ARG:HH12	1.78	0.48
63:6:59:A:H2'	63:6:60:U:H5'	1.96	0.48
65:0:468:ILE:O	65:0:472:ARG:N	2.47	0.48
4:D:12:ARG:HD3	51:1:686:U:O4	2.13	0.48
9:I:96:ARG:HH21	9:I:114:ARG:HH12	1.62	0.48
29:d:2:GLU:HB3	29:d:11:ALA:HB1	1.96	0.48
51:1:225:C:H2'	51:1:226:A:O4'	2.14	0.48
51:1:572:A:N6	51:1:2029:G:H21	2.05	0.48
51:1:639:U:H2'	51:1:640:C:C6	2.48	0.48
51:1:2221:G:O2'	51:1:2222:C:H5'	2.13	0.48
51:1:2860:A:H2'	51:1:2861:U:H5'	1.95	0.48
53:3:5:U:H4'	53:3:6:G:C8	2.49	0.48
53:3:508:U:H1'	53:3:509:A:N7	2.29	0.48
53:3:513:C:H2'	53:3:514:C:C6	2.49	0.48
53:3:631:C:H3'	53:3:632:U:H5'	1.95	0.48
53:3:1005:A:H2'	53:3:1006:G:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:A2:102:LEU:HD12	57:A2:115:ILE:HG12	1.96	0.48
58:B1:124:ILE:HG23	58:B1:128:LEU:HD12	1.94	0.48
58:B1:1146:GLU:OE2	58:B1:1310:THR:HG22	2.14	0.48
59:B2:363:LEU:HB3	59:B2:381:ALA:HB1	1.96	0.48
65:0:491:ARG:O	65:0:613:LEU:N	2.45	0.48
9:I:1:ALA:HB2	53:3:499:A:H61	1.79	0.48
16:P:121:ARG:NH2	53:3:1524:C:OP1	2.46	0.48
24:X:14:LEU:HA	24:X:17:LYS:HD2	1.96	0.48
24:X:32:THR:HG1	24:X:34:SER:HG	1.62	0.48
25:Y:20:ASN:O	25:Y:24:ARG:N	2.46	0.48
36:l:16:GLY:HA2	51:1:662:G:H5''	1.96	0.48
43:s:89:ALA:HB1	51:1:748:G:C8	2.49	0.48
51:1:1018:U:H2'	51:1:1019:U:O4'	2.13	0.48
51:1:1819:A:H4'	51:1:1820:U:H5'	1.96	0.48
53:3:714:G:H2'	53:3:715:A:O4'	2.13	0.48
53:3:1305:G:N2	53:3:1331:G:H2'	2.28	0.48
53:3:1500:A:H5''	53:3:1508:A:H5'	1.94	0.48
59:B2:529:ARG:HH11	59:B2:572:ILE:HG22	1.77	0.48
65:0:502:GLU:HA	65:0:519:VAL:HA	1.96	0.48
22:V:56:ASP:N	22:V:56:ASP:OD1	2.47	0.48
23:W:20:ILE:HD12	23:W:53:GLN:HB2	1.96	0.48
27:b:255:LYS:NZ	51:1:1844:C:H4'	2.28	0.48
48:x:57:VAL:HG22	51:1:372:G:H2'	1.96	0.48
51:1:281:C:H2'	51:1:282:A:C8	2.49	0.48
51:1:572:A:H2'	51:1:572:A:N3	2.29	0.48
51:1:2184:A:H2'	51:1:2185:U:O4'	2.13	0.48
51:1:2504:U:H2'	51:1:2505:G:H5'	1.95	0.48
52:2:5:U:H2'	52:2:6:G:C8	2.49	0.48
58:B1:190:LYS:HE3	58:B1:190:LYS:HB2	1.41	0.48
58:B1:968:ASN:HA	58:B1:1117:SER:HB2	1.96	0.48
59:B2:1311:GLY:O	60:W0:31:GLN:NE2	2.47	0.48
30:e:26:GLN:NE2	52:2:57:A:H4'	2.29	0.47
33:i:133:ARG:HB3	51:1:1077:A:O2'	2.14	0.47
48:x:22:ASN:HD22	51:1:200:U:H5'	1.79	0.47
51:1:100:U:H4'	51:1:101:A:O4'	2.14	0.47
51:1:327:G:O2'	51:1:328:U:H5'	2.14	0.47
51:1:845:A:N3	51:1:845:A:H3'	2.29	0.47
51:1:1343:G:H1'	51:1:1597:A:C4	2.49	0.47
52:2:5:U:H2'	52:2:6:G:H8	1.78	0.47
53:3:1211:U:H4'	53:3:1213:A:C4	2.48	0.47
58:B1:395:LYS:NZ	58:B1:399:LYS:CD	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:1261:LEU:HD12	58:B1:1304:ARG:HH21	1.78	0.47
59:B2:836:LEU:HD13	59:B2:1054:LEU:HD13	1.95	0.47
62:5:50:U:H2'	62:5:51:U:C6	2.49	0.47
28:c:13:ARG:NH2	28:c:21:SER:OG	2.47	0.47
31:f:44:HIS:HA	31:f:49:LEU:HD23	1.96	0.47
39:o:29:HIS:HB3	39:o:36:TYR:HB2	1.96	0.47
51:1:157:C:H2'	51:1:158:U:O4'	2.13	0.47
51:1:174:U:H2'	51:1:175:G:C8	2.49	0.47
51:1:2762:C:H2'	51:1:2763:G:H5'	1.95	0.47
53:3:505:G:OP2	53:3:535:A:H5'	2.13	0.47
53:3:994:A:C8	53:3:1216:A:H4'	2.49	0.47
58:B1:395:LYS:NZ	58:B1:399:LYS:CE	2.78	0.47
59:B2:207:THR:OG1	59:B2:354:ASP:OD2	2.32	0.47
64:a:42:VAL:HB	64:a:175:ILE:HG22	1.96	0.47
7:G:58:LYS:O	7:G:61:SER:OG	2.32	0.47
27:b:247:TRP:CD2	51:1:1805:A:H5''	2.50	0.47
33:i:55:PRO:HG2	33:i:71:LYS:HG3	1.96	0.47
51:1:419:U:H2'	51:1:420:C:C6	2.49	0.47
51:1:1533:C:C3'	51:1:1534:U:H5''	2.44	0.47
51:1:2553:G:C3'	51:1:2554:U:H5''	2.41	0.47
51:1:2637:U:H2'	51:1:2638:G:O4'	2.13	0.47
51:1:2852:G:H2'	51:1:2853:C:O4'	2.14	0.47
53:3:110:C:H2'	53:3:111:G:O4'	2.13	0.47
53:3:1527:U:O5'	53:3:1527:U:H6	1.97	0.47
55:8:15:DC:H1'	58:B1:426:ALA:HB1	1.96	0.47
59:B2:732:ILE:HD11	59:B2:769:PRO:HB3	1.95	0.47
59:B2:1286:THR:O	59:B2:1290:MET:HB2	2.14	0.47
65:0:553:VAL:HG11	65:0:578:LEU:HD22	1.96	0.47
9:I:131:ILE:HG21	53:3:620:C:O2	2.14	0.47
12:L:77:ARG:HD3	12:L:86:VAL:HG21	1.94	0.47
16:P:126:ARG:HH21	53:3:796:C:H4'	1.79	0.47
19:S:5:MET:SD	19:S:8:ARG:NH1	2.88	0.47
29:d:98:LYS:HG3	51:1:607:U:P	2.53	0.47
29:d:109:LEU:HD13	29:d:112:LEU:HD12	1.97	0.47
51:1:941:A:H2'	51:1:942:G:O4'	2.14	0.47
51:1:1018:U:H5''	51:1:1036:G:O2'	2.14	0.47
51:1:2534:A:H2'	51:1:2535:G:O4'	2.14	0.47
58:B1:1060:VAL:HG13	58:B1:1106:ILE:HG12	1.96	0.47
16:P:80:ASN:HA	16:P:104:PHE:HB3	1.96	0.47
27:b:149:LYS:HG2	27:b:152:GLN:HE22	1.80	0.47
46:v:7:GLU:HA	46:v:65:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:21:ARG:NH2	52:2:76:G:O3'	2.48	0.47
51:1:118:A:H2'	51:1:120:U:O4	2.15	0.47
51:1:609:A:H2'	51:1:610:C:O4'	2.14	0.47
51:1:1680:U:H2'	51:1:1681:G:O4'	2.15	0.47
51:1:1927:A:H2'	51:1:1928:A:C8	2.49	0.47
51:1:2818:U:H2'	51:1:2819:G:C8	2.49	0.47
53:3:110:C:H2'	53:3:111:G:C8	2.50	0.47
53:3:946:A:H2'	53:3:947:G:C8	2.49	0.47
53:3:1427:C:O2	53:3:1427:C:H2'	2.12	0.47
58:B1:1036:ARG:HE	58:B1:1081:VAL:HG11	1.79	0.47
65:0:557:ILE:HD13	65:0:576:ILE:HG12	1.96	0.47
9:I:80:ARG:NH1	53:3:613:C:OP2	2.47	0.47
14:N:113:LYS:NZ	53:3:1367:C:C6	2.83	0.47
49:y:31:GLN:HE21	49:y:36:GLN:HB2	1.80	0.47
51:1:282:A:H2'	51:1:283:G:C8	2.50	0.47
51:1:858:G:H5'	51:1:859:G:OP2	2.14	0.47
51:1:1123:C:H2'	51:1:1124:G:C8	2.49	0.47
51:1:1932:A:H2'	51:1:1933:G:O4'	2.15	0.47
51:1:2146:C:H5''	51:1:2147:A:N7	2.30	0.47
51:1:2185:U:H2'	51:1:2186:G:C8	2.48	0.47
53:3:86:G:H4'	53:3:87:C:C6	2.50	0.47
53:3:599:C:H2'	53:3:600:A:H8	1.80	0.47
58:B1:1347:LEU:HG	58:B1:1357:ILE:HG23	1.96	0.47
59:B2:133:ASN:O	59:B2:527:LYS:NZ	2.42	0.47
1:A:28:VAL:HG22	30:e:139:GLU:HA	1.96	0.47
8:H:122:GLN:HE21	8:H:127:VAL:HG21	1.80	0.47
9:I:4:LEU:HD11	53:3:405:U:C6	2.50	0.47
12:L:21:LEU:HD11	12:L:96:ASN:HD22	1.78	0.47
14:N:4:GLN:HE22	53:3:1131:G:C5'	2.25	0.47
21:U:68:SER:OG	21:U:69:ASP:OD1	2.33	0.47
21:U:69:ASP:OD1	21:U:69:ASP:N	2.48	0.47
29:d:125:SER:OG	29:d:126:VAL:N	2.48	0.47
32:g:99:ILE:O	32:g:103:VAL:N	2.40	0.47
38:n:58:ASP:OD1	38:n:63:ARG:NH2	2.48	0.47
50:z:17:PRO:HG3	51:1:969:G:OP1	2.14	0.47
51:1:41:C:C3'	51:1:42:A:H5''	2.44	0.47
51:1:552:U:H2'	51:1:553:G:H8	1.80	0.47
51:1:1409:U:H2'	51:1:1410:G:H8	1.80	0.47
51:1:1960:A:C2'	51:1:1961:C:H5''	2.44	0.47
53:3:536:C:H2'	53:3:537:G:C8	2.49	0.47
53:3:939:G:N3	53:3:1375:A:H2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:43:THR:HG22	58:B1:57:PHE:HE1	1.80	0.47
58:B1:198:CYS:HA	58:B1:221:ILE:CD1	2.45	0.47
58:B1:420:PRO:HA	58:B1:437:PHE:O	2.15	0.47
58:B1:526:VAL:HG12	58:B1:549:LYS:HB2	1.96	0.47
58:B1:833:GLU:N	58:B1:1242:ARG:HH12	2.12	0.47
62:5:26:A:N6	62:5:44:G:H1	2.13	0.47
10:J:18:ASN:OD1	10:J:33:THR:OG1	2.33	0.47
18:R:102:LYS:HE2	53:3:952:U:O4	2.14	0.47
19:S:51:PRO:O	19:S:54:SER:OG	2.31	0.47
29:d:168:ASP:OD1	29:d:168:ASP:N	2.47	0.47
36:l:89:VAL:HA	36:l:121:THR:HB	1.97	0.47
46:v:64:VAL:HA	46:v:69:GLU:HA	1.96	0.47
51:1:368:A:C2'	51:1:369:U:H5'	2.45	0.47
51:1:395:U:H2'	51:1:396:G:C8	2.50	0.47
51:1:528:A:C2	51:1:2043:C:H4'	2.50	0.47
51:1:1182:G:H2'	51:1:1183:U:O4'	2.15	0.47
53:3:202:G:H2'	53:3:203:G:C8	2.50	0.47
65:0:176:GLU:O	65:0:179:PHE:N	2.47	0.47
27:b:141:HIS:ND1	27:b:192:GLY:O	2.37	0.47
27:b:233:GLY:HA3	51:1:2598:A:H5''	1.96	0.47
39:o:94:ARG:NH2	51:1:2293:G:H5''	2.30	0.47
51:1:903:C:H2'	51:1:904:G:C8	2.49	0.47
51:1:1409:U:H2'	51:1:1410:G:C8	2.50	0.47
51:1:1906:G:C2'	51:1:1907:G:H5''	2.44	0.47
53:3:392:C:H2'	53:3:393:A:C8	2.49	0.47
53:3:935:A:H2'	53:3:936:C:C6	2.50	0.47
53:3:987:G:H2'	53:3:988:G:H8	1.80	0.47
53:3:1060:U:H2'	53:3:1061:G:C8	2.50	0.47
55:8:9:DG:H4'	58:B1:120:LEU:HG	1.97	0.47
57:A1:33:ARG:HE	57:A1:33:ARG:HB3	1.56	0.47
58:B1:1219:ASP:O	58:B1:1223:LEU:HB2	2.15	0.47
59:B2:689:ALA:HB2	59:B2:1233:LEU:HD23	1.97	0.47
30:e:140:ILE:HG22	30:e:142:TYR:H	1.80	0.47
31:f:157:LYS:HD3	31:f:157:LYS:HA	1.83	0.47
42:r:78:ARG:NH1	51:1:990:A:H61	2.13	0.47
51:1:1387:A:H5'	51:1:1469:A:H1'	1.96	0.47
51:1:1913:A:O2'	66:h:4:SER:HA	2.15	0.47
51:1:2467:C:H2'	51:1:2468:A:O4'	2.15	0.47
51:1:2653:U:C3'	51:1:2654:A:H5''	2.38	0.47
51:1:2798:U:H4'	51:1:2799:A:C4	2.50	0.47
53:3:66:A:H5''	53:3:199:A:O2'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1210:C:OP1	65:0:584:HIS:CG	2.68	0.47
58:B1:375:GLU:HB3	59:B2:1245:ALA:HB3	1.97	0.47
58:B1:842:ARG:HH22	58:B1:1250:ASP:HB2	1.80	0.47
58:B1:1357:ILE:HD13	59:B2:1279:GLU:HG2	1.97	0.47
8:H:17:TRP:O	8:H:53:ARG:NH2	2.47	0.46
14:N:4:GLN:HE22	53:3:1131:G:C4'	2.28	0.46
39:o:67:ASN:HA	52:2:50:A:OP2	2.15	0.46
42:r:7:SER:OG	42:r:8:GLY:N	2.49	0.46
51:1:76:C:H2'	51:1:77:G:H8	1.80	0.46
51:1:311:A:H3'	51:1:312:G:C8	2.49	0.46
51:1:610:C:H2'	51:1:611:C:H6	1.80	0.46
51:1:855:G:H3'	51:1:856:G:H5''	1.98	0.46
51:1:940:G:C3'	51:1:941:A:H5''	2.45	0.46
51:1:1175:A:H5'	51:1:1176:U:O4'	2.16	0.46
51:1:1300:G:H4'	51:1:1301:A:H5''	1.96	0.46
53:3:24:U:H2'	53:3:25:C:C6	2.50	0.46
53:3:177:G:O2'	53:3:1448:C:H4'	2.15	0.46
53:3:1223:C:H5	53:3:1224:U:H5	1.63	0.46
58:B1:105:ILE:HD12	58:B1:242:LEU:CD2	2.44	0.46
58:B1:108:ALA:HB1	58:B1:279:LEU:HD22	1.96	0.46
58:B1:903:LEU:HD12	58:B1:903:LEU:HA	1.81	0.46
59:B2:800:MET:HB2	59:B2:800:MET:HE3	1.69	0.46
9:I:82:LYS:HE2	53:3:3:A:OP1	2.16	0.46
15:O:42:LEU:HB3	15:O:71:LEU:HB2	1.96	0.46
25:Y:73:ARG:NE	53:3:261:U:H5	2.12	0.46
28:c:133:THR:HG22	28:c:134:HIS:H	1.80	0.46
29:d:155:GLU:HA	29:d:158:PHE:HB3	1.97	0.46
35:k:66:LYS:HD2	51:1:1665:A:H5''	1.95	0.46
37:m:31:PHE:HB3	37:m:130:PHE:HE1	1.80	0.46
39:o:30:ARG:HH21	39:o:97:PHE:HB3	1.80	0.46
41:q:105:PHE:HA	41:q:108:LEU:HD12	1.97	0.46
47:w:70:PRO:HB3	52:2:12:C:C5	2.50	0.46
51:1:479:A:H4'	51:1:480:A:H5'	1.98	0.46
51:1:1017:G:H2'	51:1:1018:U:C6	2.50	0.46
51:1:1179:G:C4	51:1:1180:U:H1'	2.50	0.46
51:1:2638:G:H1'	51:1:2778:A:N6	2.26	0.46
52:2:96:G:O2'	52:2:97:C:H5'	2.15	0.46
53:3:211:G:C2'	53:3:212:G:H5'	2.46	0.46
53:3:1382:C:O2	53:3:1382:C:O4'	2.33	0.46
58:B1:1150:PRO:HG3	58:B1:1214:PRO:HB2	1.96	0.46
62:5:8:U:H2'	62:5:13:C:N4	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:a:200:LYS:HD3	64:a:201:PRO:HD2	1.97	0.46
65:0:624:PRO:HA	65:0:651:GLY:HA2	1.97	0.46
24:X:9:PHE:CE1	53:3:1318:A:H5'	2.50	0.46
39:o:13:ARG:HH21	39:o:17:LYS:HB2	1.80	0.46
51:1:1344:U:H3'	51:1:1345:C:H5'	1.96	0.46
51:1:1717:A:H2'	51:1:1718:G:O4'	2.15	0.46
51:1:1872:A:H2'	51:1:1873:G:O4'	2.15	0.46
53:3:82:G:C2'	53:3:83:C:H5'	2.45	0.46
53:3:390:U:H2'	53:3:391:G:C8	2.50	0.46
53:3:680:C:H2'	53:3:681:A:H8	1.80	0.46
53:3:1329:A:O2'	53:3:1330:U:H5'	2.16	0.46
59:B2:562:GLU:OE1	59:B2:662:SER:OG	2.28	0.46
64:a:186:LYS:HA	64:a:189:LEU:HG	1.97	0.46
65:0:255:ARG:HD3	65:0:261:ILE:HB	1.97	0.46
12:L:26:VAL:HG22	12:L:42:VAL:HG21	1.98	0.46
14:N:70:GLY:O	14:N:74:GLN:N	2.41	0.46
21:U:68:SER:OG	21:U:69:ASP:N	2.47	0.46
27:b:46:GLY:HA3	51:1:773:U:H4'	1.97	0.46
27:b:200:MET:HE2	51:1:1820:U:C2	2.50	0.46
30:e:146:ASP:OD1	30:e:146:ASP:N	2.48	0.46
48:x:60:LYS:NZ	51:1:372:G:O4'	2.49	0.46
51:1:1023:U:H2'	51:1:1024:G:H5'	1.97	0.46
51:1:2126:A:C2'	51:1:2162:G:H21	2.29	0.46
53:3:479:U:H2'	53:3:480:U:H5'	1.96	0.46
58:B1:352:ARG:CD	59:B2:1268:GLN:NE2	2.67	0.46
59:B2:230:PHE:HB2	59:B2:333:ILE:HB	1.97	0.46
65:0:592:ALA:O	65:0:596:ALA:N	2.46	0.46
8:H:23:ALA:HB1	8:H:27:GLU:HG2	1.97	0.46
17:Q:68:GLY:O	53:3:521:G:H5'	2.15	0.46
25:Y:9:ARG:NH1	53:3:107:G:O6	2.49	0.46
27:b:48:ILE:HG22	51:1:779:U:P	2.55	0.46
27:b:140:VAL:HG23	27:b:161:VAL:HG13	1.96	0.46
47:w:38:GLY:CA	51:1:2330:G:H21	2.26	0.46
51:1:337:C:H2'	51:1:338:G:O4'	2.15	0.46
51:1:562:U:O4'	51:1:2036:C:H5'	2.16	0.46
51:1:2898:U:H2'	51:1:2899:A:C8	2.51	0.46
53:3:490:C:H2'	53:3:491:G:C8	2.49	0.46
53:3:864:A:H2'	53:3:865:A:C8	2.51	0.46
53:3:1369:C:H2'	53:3:1370:G:C8	2.49	0.46
53:3:1497:G:C2'	53:3:1498:U:H5'	2.46	0.46
58:B1:29:MET:HG2	59:B2:1336:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:1027:VAL:HB	58:B1:1121:LEU:HB2	1.95	0.46
59:B2:400:VAL:HG22	59:B2:584:TYR:HB3	1.96	0.46
59:B2:1314:GLN:HA	60:W0:28:ARG:HH22	1.80	0.46
12:L:71:THR:O	12:L:90:VAL:HG22	2.16	0.46
13:M:9:MET:HB2	13:M:32:LYS:HE2	1.96	0.46
27:b:54:GLY:HA3	27:b:216:ARG:HG3	1.98	0.46
51:1:416:U:H3	51:1:2407:A:H61	1.63	0.46
51:1:621:A:H2'	51:1:622:G:O4'	2.15	0.46
51:1:2066:C:O2'	51:1:2067:G:H5'	2.16	0.46
51:1:2126:A:H5'	51:1:2127:G:O5'	2.16	0.46
53:3:31:G:N2	53:3:47:C:H5''	2.31	0.46
53:3:1137:C:H5'	53:3:1138:G:H5'	1.97	0.46
54:4:5:U:H2'	54:4:6:U:C6	2.50	0.46
57:A2:64:VAL:HG11	57:A2:78:ILE:HG21	1.97	0.46
58:B1:1167:LYS:NZ	58:B1:1170:LYS:HB2	2.30	0.46
59:B2:517:GLN:HB3	59:B2:760:ASN:H	1.79	0.46
64:a:69:THR:HA	64:a:176:GLY:HA2	1.97	0.46
65:0:515:TYR:HB3	65:0:584:HIS:CB	2.44	0.46
1:A:53:THR:OG1	1:A:54:GLY:N	2.49	0.46
1:A:63:ARG:HD2	53:3:1012:A:OP2	2.16	0.46
12:L:111:GLY:HA2	12:L:118:ARG:HD3	1.97	0.46
14:N:128:LYS:HE3	63:6:34:C:OP2	2.16	0.46
27:b:141:HIS:N	27:b:190:THR:O	2.46	0.46
33:i:129:GLU:HB2	33:i:139:VAL:HG21	1.98	0.46
51:1:1335:C:H2'	51:1:1336:A:H8	1.80	0.46
51:1:2849:U:H4'	51:1:2868:A:C2	2.50	0.46
53:3:194:C:O2'	53:3:195:A:H5'	2.15	0.46
58:B1:1221:LEU:HD22	58:B1:1306:LEU:HB2	1.96	0.46
62:5:8:U:H2'	62:5:13:C:H41	1.81	0.46
65:0:20:ASP:HA	68:0:801:GDP:H5'	1.96	0.46
65:0:536:PHE:HD1	65:0:576:ILE:HG23	1.81	0.46
8:H:176:THR:HG22	8:H:179:ALA:H	1.81	0.46
12:L:87:PRO:HG3	12:L:148:LYS:HA	1.98	0.46
24:X:79:TYR:CZ	53:3:1226:C:H4'	2.51	0.46
32:g:103:VAL:O	32:g:107:GLY:N	2.49	0.46
42:r:85:LYS:HA	51:1:814:C:OP1	2.16	0.46
51:1:1557:C:H3'	51:1:1558:C:C5'	2.31	0.46
51:1:1709:U:H2'	51:1:1710:G:C8	2.51	0.46
51:1:1842:G:H2'	51:1:1843:C:O4'	2.16	0.46
51:1:2176:A:H5'	64:a:219:GLY:O	2.16	0.46
51:1:2385:C:H2'	51:1:2386:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2644:G:C2'	51:1:2645:G:H5'	2.46	0.46
52:2:43:C:H2'	52:2:44:G:H5''	1.97	0.46
53:3:70:U:H4'	53:3:71:A:C8	2.51	0.46
53:3:91:U:C2'	53:3:92:U:H5''	2.45	0.46
53:3:253:A:H2'	53:3:254:G:H8	1.81	0.46
53:3:629:A:H2'	53:3:630:A:O4'	2.15	0.46
57:A1:185:TYR:HA	57:A1:202:VAL:O	2.16	0.46
58:B1:128:LEU:HD21	58:B1:188:LEU:HB3	1.97	0.46
58:B1:343:LEU:HD11	58:B1:1324:SER:HB3	1.97	0.46
58:B1:352:ARG:HB2	59:B2:1268:GLN:NE2	2.30	0.46
6:F:29:ALA:O	31:f:169:ARG:NH1	2.44	0.46
9:I:61:ARG:HH12	9:I:68:GLU:N	2.13	0.46
21:U:5:ARG:HD2	53:3:376:G:H4'	1.97	0.46
38:n:64:ARG:HH11	51:1:2705:A:H2	1.63	0.46
51:1:341:C:H2'	51:1:342:A:H8	1.80	0.46
51:1:610:C:H2'	51:1:611:C:C6	2.50	0.46
51:1:1000:A:H2'	51:1:1001:A:C8	2.51	0.46
51:1:1433:A:H2'	51:1:1434:A:O4'	2.16	0.46
51:1:1638:C:H5''	51:1:2710:C:O2'	2.16	0.46
51:1:2670:A:H2'	51:1:2671:G:H8	1.81	0.46
51:1:2804:U:H2'	51:1:2805:C:C6	2.51	0.46
53:3:1268:G:H21	53:3:1327:C:H1'	1.80	0.46
57:A1:35:PHE:HA	57:A1:38:THR:HG22	1.97	0.46
57:A2:80:GLU:HG3	59:B2:694:ARG:HH22	1.81	0.46
58:B1:115:TRP:HB3	58:B1:1333:THR:CG2	2.46	0.46
58:B1:891:ASP:OD2	58:B1:1290:ARG:NH2	2.47	0.46
59:B2:148:GLN:NE2	59:B2:535:PRO:O	2.40	0.46
14:N:108:ARG:O	53:3:1347:G:H8	1.99	0.46
16:P:17:ASP:N	16:P:17:ASP:OD1	2.49	0.46
18:R:97:ARG:HG3	53:3:1308:U:OP2	2.16	0.46
18:R:100:ARG:HH21	18:R:102:LYS:HD3	1.81	0.46
19:S:92:ILE:HD13	19:S:95:LEU:HD12	1.97	0.46
33:i:11:GLN:HG2	33:i:23:VAL:HG11	1.98	0.46
34:j:80:HIS:CD2	51:1:2642:G:H5'	2.51	0.46
42:r:81:LYS:HD3	51:1:973:A:H5''	1.98	0.46
51:1:687:C:H2'	51:1:688:U:O4'	2.16	0.46
51:1:863:A:H4'	52:2:100:G:N2	2.31	0.46
51:1:1015:U:H2'	51:1:1016:G:C8	2.51	0.46
51:1:1112:G:O2'	51:1:1113:U:H5'	2.15	0.46
51:1:2189:U:H2'	51:1:2190:G:C8	2.51	0.46
51:1:2649:C:H2'	51:1:2650:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2811:G:H2'	51:1:2812:G:C8	2.51	0.46
53:3:312:C:H2'	53:3:313:A:C8	2.51	0.46
53:3:408:A:H2'	53:3:409:U:O4'	2.16	0.46
57:A1:212:ASP:OD1	57:A1:212:ASP:N	2.48	0.46
58:B1:288:PRO:HB3	61:NG:105:ASP:H	1.80	0.46
58:B1:772:TYR:HE2	59:B2:561:ILE:HG21	1.80	0.46
65:0:33:TYR:HE2	65:0:275:VAL:HB	1.81	0.46
9:I:72:ARG:HG2	9:I:76:LYS:HE3	1.97	0.45
14:N:86:LEU:HD13	14:N:93:LEU:HD22	1.97	0.45
16:P:123:PRO:O	26:Z:34:ARG:N	2.40	0.45
27:b:200:MET:HE2	51:1:1820:U:N3	2.31	0.45
30:e:12:VAL:HG13	30:e:27:VAL:HG11	1.98	0.45
41:q:92:LYS:NZ	51:1:995:C:O2'	2.44	0.45
44:t:2:ILE:HG13	44:t:5:GLU:HB3	1.98	0.45
51:1:878:A:H3'	51:1:879:G:C8	2.51	0.45
51:1:1822:C:H2'	51:1:1823:G:H8	1.81	0.45
51:1:2211:A:H5'	51:1:2212:A:OP2	2.16	0.45
53:3:51:A:H4'	53:3:52:C:H5''	1.98	0.45
53:3:401:C:H2'	53:3:402:G:H8	1.81	0.45
53:3:448:A:H3'	53:3:449:G:C8	2.51	0.45
53:3:1342:C:H2'	53:3:1343:G:C8	2.51	0.45
58:B1:141:PHE:CE2	58:B1:296:LYS:CB	2.94	0.45
58:B1:209:ASN:HA	58:B1:214:ARG:NH2	2.31	0.45
58:B1:385:LEU:HD23	58:B1:390:LEU:HB2	1.98	0.45
59:B2:28:LEU:HD21	59:B2:524:ILE:HG13	1.98	0.45
59:B2:735:LYS:HA	59:B2:748:ILE:HG22	1.97	0.45
62:5:70:G:H2'	62:5:71:G:C8	2.51	0.45
17:Q:14:LYS:HE3	53:3:884:U:O2'	2.15	0.45
24:X:5:LYS:HG2	53:3:1313:U:P	2.56	0.45
25:Y:28:ARG:HD3	53:3:1438:G:OP1	2.16	0.45
33:i:124:MET:HE3	33:i:124:MET:HB3	1.70	0.45
39:o:27:VAL:HG12	39:o:93:ASP:HB3	1.98	0.45
43:s:33:LEU:O	43:s:37:THR:OG1	2.33	0.45
46:v:30:ILE:HG12	46:v:91:PHE:HB2	1.96	0.45
51:1:1424:G:H2'	51:1:1425:G:O4'	2.17	0.45
51:1:2174:C:O2'	64:a:218:MET:HG2	2.17	0.45
51:1:2773:C:H2'	51:1:2774:C:C6	2.51	0.45
51:1:2800:A:H3'	51:1:2801:G:C5'	2.45	0.45
52:2:49:C:H2'	52:2:50:A:C8	2.49	0.45
52:2:97:C:H2'	52:2:98:G:C5'	2.46	0.45
53:3:555:U:H2'	53:3:556:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:652:U:H2'	53:3:653:U:H5''	1.98	0.45
58:B1:375:GLU:O	59:B2:1247:SER:HB3	2.16	0.45
59:B2:103:VAL:HG12	59:B2:117:ILE:HG22	1.97	0.45
65:0:131:ASN:OD1	65:0:137:ARG:NH2	2.50	0.45
65:0:523:TYR:HD2	65:0:577:ARG:HH12	1.63	0.45
5:E:3:ILE:HD11	51:1:592:A:C2	2.51	0.45
12:L:67:ASN:O	12:L:137:ARG:NH1	2.49	0.45
51:1:676:A:H62	51:1:802:A:H61	1.63	0.45
51:1:677:A:O2'	51:1:2071:A:H5'	2.16	0.45
51:1:933:A:H5''	51:1:934:U:H5	1.81	0.45
51:1:2468:A:O2'	51:1:2469:A:H5'	2.16	0.45
53:3:485:U:H5'	53:3:486:U:OP2	2.16	0.45
53:3:1107:C:O2'	53:3:1191:A:H4'	2.16	0.45
53:3:1146:A:H2'	53:3:1147:C:H5'	1.97	0.45
53:3:1149:C:O2'	53:3:1150:A:H5'	2.17	0.45
53:3:1275:A:N1	53:3:1283:U:H5'	2.31	0.45
56:9:27:DC:P	59:B2:542:ARG:HE	2.39	0.45
58:B1:75:TYR:CD2	58:B1:75:TYR:O	2.70	0.45
58:B1:1227:HIS:HA	58:B1:1230:THR:HG22	1.99	0.45
65:0:149:ALA:N	65:0:176:GLU:OE1	2.43	0.45
9:I:173:ASP:HB3	9:I:178:GLU:H	1.82	0.45
17:Q:106:VAL:HG23	17:Q:116:TYR:HB3	1.98	0.45
24:X:36:ARG:HB3	53:3:1320:C:N4	2.30	0.45
28:c:56:LYS:HZ1	51:1:2830:C:H5''	1.81	0.45
38:n:39:PRO:HG3	51:1:1651:G:C5'	2.46	0.45
40:p:22:GLY:H	40:p:46:VAL:HG23	1.80	0.45
41:q:74:SER:OG	41:q:75:TYR:N	2.49	0.45
50:z:40:THR:HG23	50:z:42:ALA:H	1.80	0.45
51:1:209:C:H4'	51:1:681:G:H4'	1.97	0.45
51:1:979:A:H2'	51:1:982:C:H42	1.81	0.45
51:1:2190:G:O2'	51:1:2191:A:H5'	2.16	0.45
52:2:66:A:N1	52:2:107:G:H2'	2.31	0.45
53:3:1005:A:H2'	53:3:1006:G:O4'	2.16	0.45
53:3:1414:U:H2'	53:3:1415:G:H8	1.81	0.45
58:B1:68:TYR:HB3	58:B1:75:TYR:HE2	1.81	0.45
58:B1:109:SER:HB2	58:B1:296:LYS:HG2	1.98	0.45
58:B1:506:VAL:HG23	58:B1:628:GLY:HA3	1.99	0.45
58:B1:1158:GLU:HA	58:B1:1223:LEU:HD21	1.99	0.45
59:B2:24:VAL:HG11	59:B2:704:MET:HE1	1.98	0.45
60:W0:25:ARG:NH1	60:W0:61:ASN:OD1	2.49	0.45
62:5:6:G:H2'	62:5:7:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:0:305:THR:O	65:0:305:THR:OG1	2.34	0.45
11:K:49:TYR:HB3	23:W:73:HIS:CG	2.52	0.45
12:L:115:MET:HA	12:L:118:ARG:HB2	1.98	0.45
15:O:6:ILE:HD12	15:O:102:LEU:HG	1.97	0.45
31:f:21:GLN:OE1	31:f:54:ARG:NH2	2.39	0.45
40:p:27:VAL:HG13	40:p:42:PHE:HB3	1.98	0.45
51:1:195:A:H3'	51:1:196:A:H4'	1.99	0.45
51:1:207:A:H2'	51:1:208:C:O4'	2.16	0.45
51:1:700:G:O2'	51:1:701:G:H5'	2.17	0.45
51:1:863:A:H2'	51:1:864:G:C8	2.51	0.45
51:1:894:U:H2'	51:1:895:U:O4'	2.16	0.45
51:1:1558:C:H6	51:1:1558:C:OP1	1.98	0.45
51:1:2573:C:H5''	51:1:2574:G:H5''	1.98	0.45
53:3:974:A:H5'	53:3:976:G:OP1	2.17	0.45
57:A1:59:VAL:HG22	57:A1:144:ILE:HA	1.97	0.45
65:0:15:ILE:HG13	65:0:110:VAL:HB	1.99	0.45
65:0:602:LYS:HD3	65:0:602:LYS:HA	1.82	0.45
65:0:667:ALA:HB2	65:0:680:TYR:HE1	1.80	0.45
25:Y:2:ASN:N	53:3:332:G:OP2	2.49	0.45
37:m:2:LEU:HD23	37:m:2:LEU:HA	1.85	0.45
39:o:24:THR:HB	39:o:42:PRO:HG3	1.97	0.45
51:1:999:U:O2'	51:1:1000:A:H5'	2.16	0.45
51:1:2146:C:H5''	51:1:2147:A:C8	2.51	0.45
51:1:2799:A:C2'	51:1:2800:A:H5'	2.44	0.45
53:3:315:A:H5''	53:3:317:U:OP2	2.17	0.45
53:3:350:G:H2'	53:3:351:G:C8	2.52	0.45
53:3:405:U:C3'	53:3:406:G:H5'	2.40	0.45
53:3:990:C:H2'	53:3:991:U:O4'	2.16	0.45
53:3:1306:A:C2	53:3:1332:A:H1'	2.52	0.45
65:0:11:ARG:NH1	65:0:288:SER:OG	2.50	0.45
3:C:35:LEU:HD11	51:1:2286:G:N1	2.31	0.45
9:I:24:VAL:H	53:3:409:U:H5''	1.82	0.45
12:L:9:ARG:NH2	53:3:1346:A:C8	2.85	0.45
26:Z:66:ARG:HD2	53:3:1099:G:H4'	1.99	0.45
27:b:237:ARG:NH1	51:1:2590:A:O3'	2.49	0.45
51:1:90:U:H2'	51:1:91:A:C8	2.51	0.45
51:1:634:C:H2'	51:1:635:C:C6	2.52	0.45
51:1:1011:G:H1'	51:1:1013:C:O4'	2.16	0.45
51:1:1697:G:H3'	51:1:1698:A:C5'	2.36	0.45
51:1:1758:U:C5	51:1:2696:U:H5'	2.51	0.45
51:1:1934:C:H4'	51:1:1974:C:O3'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2472:G:O6	51:1:2476:A:H4'	2.16	0.45
53:3:451:A:N6	53:3:480:U:H2'	2.32	0.45
53:3:819:A:H5'	53:3:820:U:H5	1.82	0.45
53:3:1202:U:H2'	53:3:1203:C:O4'	2.16	0.45
53:3:1449:C:O2'	53:3:1450:U:H5'	2.16	0.45
57:A1:231:PHE:O	57:A2:218:ARG:NH1	2.49	0.45
58:B1:484:MET:CE	59:B2:1278:LEU:HD21	2.46	0.45
59:B2:1002:LEU:HD21	59:B2:1007:LYS:HB2	1.98	0.45
8:H:15:LYS:HD2	8:H:15:LYS:HA	1.81	0.45
10:J:107:GLY:CA	53:3:8:A:H1'	2.46	0.45
24:X:53:GLY:HA3	53:3:958:A:H61	1.81	0.45
27:b:204:LEU:HD21	27:b:213:ARG:HH21	1.82	0.45
28:c:173:GLN:NE2	51:1:2771:C:O2'	2.50	0.45
33:i:34:ILE:O	33:i:38:CYS:N	2.49	0.45
33:i:120:ASP:O	33:i:123:ALA:N	2.49	0.45
38:n:21:PHE:HB3	38:n:47:VAL:HG21	1.99	0.45
51:1:133:U:H2'	51:1:134:G:C8	2.52	0.45
51:1:748:G:H2'	51:1:750:A:OP2	2.17	0.45
51:1:1102:C:H2'	51:1:1103:A:O4'	2.16	0.45
51:1:2093:G:N7	51:1:2225:A:H2'	2.31	0.45
51:1:2332:C:H2'	51:1:2335:A:N3	2.31	0.45
51:1:2843:G:O2'	51:1:2844:G:H5'	2.17	0.45
58:B1:201:LEU:CD1	58:B1:224:LEU:HD12	2.46	0.45
58:B1:388:ARG:HG2	58:B1:388:ARG:NH1	2.32	0.45
58:B1:770:LEU:HD13	59:B2:618:GLN:CD	2.42	0.45
59:B2:176:ILE:HD11	59:B2:428:VAL:HG21	1.98	0.45
59:B2:746:ALA:O	59:B2:974:ARG:NH2	2.45	0.45
6:F:4:ARG:NH1	6:F:35:GLN:OE1	2.50	0.45
7:G:20:ARG:H	7:G:20:ARG:HG3	1.50	0.45
11:K:38:ARG:HB2	11:K:63:ASN:HB2	1.98	0.45
25:Y:73:ARG:CZ	53:3:261:U:C5	2.98	0.45
28:c:109:VAL:HG11	28:c:193:VAL:HB	1.99	0.45
38:n:106:ASP:N	38:n:106:ASP:OD1	2.47	0.45
50:z:27:GLY:HA3	50:z:37:ARG:HH21	1.81	0.45
51:1:300:A:C5	51:1:334:C:H4'	2.52	0.45
51:1:322:A:H5'	51:1:340:A:C1'	2.46	0.45
51:1:519:U:H2'	51:1:520:G:H8	1.82	0.45
51:1:828:U:H2'	51:1:829:A:C8	2.51	0.45
51:1:1637:A:H4'	51:1:2711:A:O2'	2.16	0.45
51:1:1725:U:H2'	51:1:1726:C:C6	2.51	0.45
51:1:2215:C:H2'	51:1:2216:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2646:C:H2'	51:1:2647:U:O4'	2.17	0.45
53:3:820:U:H3'	53:3:821:G:C5'	2.47	0.45
53:3:1005:A:C2'	53:3:1006:G:H5'	2.46	0.45
58:B1:472:LEU:CD1	59:B2:1294:LYS:HG2	2.47	0.45
58:B1:1167:LYS:HZ2	58:B1:1170:LYS:HB2	1.81	0.45
59:B2:712:SER:OG	59:B2:713:GLY:N	2.49	0.45
62:5:69:G:H2'	62:5:70:G:C8	2.52	0.45
29:d:111:GLU:OE1	29:d:114:ARG:NH2	2.50	0.45
42:r:85:LYS:HE3	51:1:815:C:P	2.57	0.45
51:1:2123:G:H2'	51:1:2124:G:C8	2.52	0.45
51:1:2206:C:H2'	51:1:2207:C:C6	2.52	0.45
53:3:303:A:H2'	53:3:304:U:O4'	2.17	0.45
53:3:495:A:H4'	53:3:496:A:H5'	1.99	0.45
53:3:556:C:H2'	53:3:557:G:O4'	2.17	0.45
53:3:596:A:H5'	53:3:596:A:H8	1.82	0.45
53:3:1261:A:H5''	53:3:1262:C:H5	1.82	0.45
55:8:1:DC:H2''	55:8:2:DC:C6	2.51	0.45
58:B1:213:LYS:HA	58:B1:213:LYS:HE3	1.99	0.45
58:B1:847:ASP:N	58:B1:847:ASP:OD1	2.49	0.45
62:5:33:U:H6	62:5:36:A:H8	1.65	0.45
9:I:141:VAL:HG23	9:I:180:THR:HG22	1.99	0.44
31:f:120:ILE:HG22	31:f:134:GLY:HA3	2.00	0.44
41:q:32:ARG:HB2	51:1:581:C:OP1	2.16	0.44
43:s:25:ARG:HE	43:s:74:ILE:HG23	1.82	0.44
44:t:30:ILE:HG23	44:t:85:VAL:HB	1.99	0.44
51:1:275:C:H2'	51:1:276:U:H4'	1.98	0.44
51:1:503:A:H5''	51:1:505:A:OP1	2.17	0.44
51:1:1528:A:H2'	51:1:1529:G:O4'	2.16	0.44
51:1:1716:U:H2'	51:1:1717:A:H8	1.81	0.44
51:1:2177:C:H1'	64:a:172:HIS:NE2	2.32	0.44
51:1:2554:U:H2'	51:1:2555:U:C6	2.52	0.44
53:3:169:C:H2'	53:3:170:U:C5	2.52	0.44
53:3:513:C:H2'	53:3:514:C:H6	1.82	0.44
53:3:884:U:H4'	53:3:885:G:C5'	2.43	0.44
53:3:1209:C:H2'	53:3:1210:C:C6	2.52	0.44
53:3:1289:A:H2'	53:3:1290:G:H5'	1.99	0.44
58:B1:804:ALA:HB2	58:B1:1256:ILE:CD1	2.48	0.44
66:h:2:DPP:NG	66:h:3:SER:N	2.65	0.44
8:H:122:GLN:O	8:H:125:ARG:HB2	2.17	0.44
18:R:26:LYS:O	18:R:30:LYS:NZ	2.44	0.44
20:T:49:HIS:CD2	53:3:764:C:H5''	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:46:GLY:HA3	51:1:773:U:H5'	2.00	0.44
27:b:58:LYS:HB3	51:1:1568:G:H4'	1.98	0.44
31:f:41:GLU:HA	31:f:54:ARG:HH21	1.81	0.44
33:i:5:GLN:H	33:i:5:GLN:HG3	1.54	0.44
35:k:97:THR:OG1	35:k:98:ARG:N	2.51	0.44
36:l:110:VAL:HB	36:l:127:VAL:HG13	1.99	0.44
51:1:311:A:H3'	51:1:312:G:H8	1.82	0.44
51:1:942:G:H2'	51:1:943:A:O4'	2.16	0.44
51:1:1748:C:H2'	51:1:1749:A:C8	2.52	0.44
51:1:2443:C:O2'	51:1:2444:G:H5'	2.17	0.44
51:1:2515:C:H2'	51:1:2516:A:H8	1.81	0.44
51:1:2670:A:H2'	51:1:2671:G:C8	2.53	0.44
53:3:29:U:H5'	53:3:296:U:OP1	2.17	0.44
53:3:993:G:N3	53:3:993:G:H2'	2.32	0.44
53:3:1222:G:O2'	53:3:1223:C:H5'	2.17	0.44
58:B1:67:ASP:OD1	58:B1:67:ASP:O	2.35	0.44
58:B1:1357:ILE:HG22	58:B1:1359:ALA:H	1.83	0.44
59:B2:11:ILE:HG22	59:B2:1172:LEU:HD11	1.99	0.44
62:5:49:C:H2'	62:5:50:U:C6	2.52	0.44
1:A:58:ASP:HB2	24:X:20:LYS:HB2	1.99	0.44
3:C:29:LYS:HE2	51:1:2286:G:H3'	1.99	0.44
9:I:90:LEU:HD13	9:I:190:LEU:HD11	1.98	0.44
16:P:117:HIS:CD2	53:3:675:A:H1'	2.52	0.44
27:b:17:LYS:HE3	27:b:17:LYS:HB2	1.83	0.44
28:c:103:ASP:OD1	28:c:103:ASP:N	2.49	0.44
28:c:114:LYS:HD2	51:1:2820:A:O2'	2.18	0.44
51:1:864:G:O2'	51:1:865:C:H5'	2.17	0.44
51:1:1363:C:O2'	51:1:1364:G:H5'	2.18	0.44
53:3:1042:A:H2'	53:3:1043:G:H1'	1.99	0.44
58:B1:45:ASN:HD22	58:B1:48:THR:H	1.65	0.44
58:B1:731:ARG:HB3	59:B2:1105:SER:HB2	2.00	0.44
59:B2:674:ASP:OD2	59:B2:1070:HIS:ND1	2.50	0.44
65:0:169:LEU:HG	65:0:263:LEU:HB3	1.99	0.44
30:e:70:ARG:HH12	30:e:71:LYS:HE3	1.82	0.44
36:l:63:LYS:HE2	51:1:249:C:O2'	2.17	0.44
38:n:42:LYS:HG2	38:n:45:ARG:HH21	1.82	0.44
41:q:2:ARG:HH11	51:1:449:A:H4'	1.81	0.44
45:u:81:ARG:HD3	51:1:335:C:H5''	1.98	0.44
51:1:367:G:O2'	51:1:368:A:H5'	2.18	0.44
51:1:716:A:C2	51:1:717:C:H1'	2.52	0.44
51:1:1064:C:C3'	51:1:1065:U:C5'	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1822:C:H2'	51:1:1823:G:C8	2.53	0.44
51:1:2189:U:H2'	51:1:2190:G:H8	1.83	0.44
51:1:2654:A:H8	51:1:2654:A:OP1	2.01	0.44
53:3:1268:G:H21	53:3:1327:C:C1'	2.29	0.44
57:A1:29:GLU:HB3	57:A1:200:LYS:HG3	1.98	0.44
58:B1:161:THR:H	58:B1:164:GLN:HB2	1.82	0.44
58:B1:395:LYS:NZ	58:B1:399:LYS:HE2	2.32	0.44
58:B1:434:ILE:HD11	59:B2:1274:GLU:HG3	2.00	0.44
62:5:13:C:H42	62:5:46:G:N2	2.15	0.44
64:a:46:VAL:HG22	64:a:212:VAL:HG13	1.99	0.44
65:0:491:ARG:HD2	65:0:570:PRO:HB2	1.99	0.44
65:0:514:GLN:HA	65:0:587:ASP:HB3	1.99	0.44
15:O:64:GLN:NE2	53:3:1368:A:OP1	2.51	0.44
38:n:35:LYS:NZ	38:n:100:CYS:SG	2.91	0.44
41:q:23:TYR:HB2	41:q:28:SER:HB3	1.98	0.44
51:1:20:C:H2'	51:1:21:A:H8	1.81	0.44
51:1:1595:C:H2'	51:1:1596:A:C8	2.52	0.44
53:3:163:C:H2'	53:3:164:G:O4'	2.17	0.44
57:A1:192:VAL:HG12	57:A1:193:GLU:H	1.83	0.44
58:B1:175:GLU:H	58:B1:175:GLU:HG3	1.66	0.44
59:B2:1246:ARG:HH11	59:B2:1266:GLY:HA2	1.82	0.44
64:a:65:LEU:HD13	64:a:188:ASN:HD21	1.83	0.44
64:a:173:THR:HG22	64:a:174:THR:H	1.82	0.44
65:0:99:VAL:HG11	65:0:126:VAL:HG12	1.99	0.44
65:0:498:VAL:HG11	65:0:522:MET:H	1.82	0.44
1:A:46:GLY:HA2	1:A:49:ARG:HG2	1.98	0.44
1:A:59:ARG:HD3	24:X:20:LYS:HE3	1.99	0.44
7:G:218:ALA:HA	7:G:221:ARG:HD3	2.00	0.44
14:N:114:LYS:HB2	14:N:117:LEU:HB2	1.99	0.44
35:k:8:LEU:HD23	35:k:82:ASN:HB3	2.00	0.44
44:t:11:LEU:O	49:y:29:ARG:NH2	2.50	0.44
51:1:19:A:O2'	51:1:553:G:H4'	2.18	0.44
51:1:974:G:H1'	51:1:975:A:H8	1.78	0.44
51:1:1075:C:H3'	51:1:1076:C:C5'	2.40	0.44
51:1:2157:G:H5''	51:1:2158:A:OP1	2.17	0.44
51:1:2457:U:O2'	51:1:2458:G:H5'	2.18	0.44
51:1:2798:U:H4'	51:1:2799:A:C5	2.53	0.44
53:3:357:G:OP1	53:3:367:U:H2'	2.17	0.44
53:3:667:G:H2'	53:3:668:G:H8	1.83	0.44
58:B1:68:TYR:O	58:B1:75:TYR:CD2	2.70	0.44
58:B1:201:LEU:HD11	58:B1:220:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:213:LYS:HE3	58:B1:213:LYS:CA	2.47	0.44
58:B1:1033:GLY:HA3	58:B1:1081:VAL:O	2.18	0.44
58:B1:1108:GLN:HG3	58:B1:1109:LEU:HD12	1.99	0.44
14:N:64:ILE:HG21	14:N:78:ILE:HG12	1.98	0.44
27:b:255:LYS:HZ3	51:1:1844:C:H4'	1.81	0.44
28:c:56:LYS:NZ	51:1:2830:C:H5''	2.33	0.44
28:c:109:VAL:HG13	28:c:201:LEU:HD13	1.99	0.44
45:u:17:ASP:HB3	45:u:20:LYS:HD2	2.00	0.44
51:1:861:A:H2'	51:1:862:G:O4'	2.18	0.44
51:1:892:A:O2'	51:1:893:C:H5'	2.17	0.44
51:1:1319:C:O2'	51:1:1320:C:H5'	2.18	0.44
51:1:2303:G:O2'	51:1:2304:G:H5'	2.17	0.44
53:3:212:G:H2'	53:3:213:G:O4'	2.17	0.44
53:3:288:A:H2'	53:3:289:G:H4'	1.99	0.44
53:3:443:C:H2'	53:3:444:G:C8	2.53	0.44
58:B1:107:LEU:HA	58:B1:276:ASN:ND2	2.33	0.44
58:B1:126:LEU:H	58:B1:126:LEU:HG	1.67	0.44
59:B2:557:ARG:HB3	59:B2:587:LEU:HD13	2.00	0.44
59:B2:557:ARG:NH2	59:B2:607:SER:O	2.49	0.44
64:a:9:ARG:HA	64:a:12:ARG:HB2	1.99	0.44
65:0:70:ALA:O	65:0:84:ILE:N	2.46	0.44
65:0:75:MET:HE1	65:0:276:GLN:HB3	1.99	0.44
4:D:8:SER:OG	51:1:686:U:O2	2.36	0.44
10:J:55:VAL:HB	10:J:56:PRO:HD3	2.00	0.44
12:L:91:ARG:HB3	12:L:92:PRO:HD2	1.99	0.44
15:O:92:LEU:HD12	15:O:92:LEU:HA	1.75	0.44
15:O:94:ALA:C	15:O:96:VAL:N	2.75	0.44
20:T:46:LYS:C	20:T:48:ASP:H	2.26	0.44
27:b:42:ARG:HH12	51:1:779:U:H5''	1.82	0.44
28:c:32:ASN:O	28:c:96:ILE:N	2.50	0.44
30:e:39:VAL:HG12	30:e:41:GLU:H	1.82	0.44
34:j:6:ALA:HB3	34:j:48:VAL:HG21	1.99	0.44
37:m:74:THR:OG1	37:m:75:GLU:N	2.50	0.44
38:n:83:LEU:HG	38:n:86:ARG:HH21	1.83	0.44
51:1:41:C:C2'	51:1:42:A:H5''	2.45	0.44
51:1:48:G:O3'	51:1:51:G:H5'	2.17	0.44
51:1:1468:U:H2'	51:1:1522:A:N6	2.33	0.44
51:1:1469:A:H2'	51:1:1470:A:C8	2.52	0.44
51:1:2039:U:H2'	51:1:2040:G:H8	1.83	0.44
51:1:2070:A:O2'	51:1:2071:A:H5'	2.17	0.44
52:2:75:G:H2'	52:2:76:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:410:G:C6	53:3:429:U:H1'	2.53	0.44
53:3:961:U:H2'	53:3:962:C:O4'	2.18	0.44
53:3:1270:G:H2'	53:3:1271:A:C8	2.53	0.44
58:B1:33:TRP:HZ2	59:B2:1336:ASN:OD1	2.00	0.44
58:B1:478:LEU:HD21	60:W0:47:THR:HG23	1.99	0.44
59:B2:862:LEU:HB2	59:B2:865:LEU:HG	2.00	0.44
65:0:537:ILE:HB	65:0:577:ARG:HG3	1.99	0.44
7:G:87:ASP:OD1	7:G:87:ASP:N	2.51	0.44
7:G:160:LEU:HD11	7:G:175:ALA:HB2	1.98	0.44
8:H:71:ARG:HD3	59:B2:859:GLU:HG3	1.99	0.44
9:I:131:ILE:HD13	53:3:620:C:C2	2.52	0.44
9:I:184:LYS:HE3	9:I:184:LYS:HB3	1.77	0.44
10:J:131:ASN:ND2	53:3:18:C:H5''	2.33	0.44
17:Q:93:ARG:NH1	53:3:911:U:OP2	2.51	0.44
19:S:74:ARG:NH2	53:3:1359:C:H3'	2.32	0.44
22:V:18:LYS:HE2	53:3:255:G:H4'	1.99	0.44
37:m:34:LYS:HE3	37:m:131:VAL:HG11	1.98	0.44
51:1:2358:A:H2'	51:1:2359:C:O4'	2.18	0.44
53:3:16:A:O2'	53:3:17:U:H5'	2.18	0.44
55:8:16:DT:H2'	55:8:17:DC:C6	2.52	0.44
57:A1:78:ILE:HA	57:A1:81:ILE:HG22	2.00	0.44
58:B1:1046:ILE:HG22	58:B1:1061:VAL:HA	2.00	0.44
59:B2:871:VAL:HG22	59:B2:872:TYR:H	1.82	0.44
2:B:42:ILE:HG12	38:n:100:CYS:HA	1.99	0.43
7:G:110:ILE:O	7:G:114:LYS:N	2.51	0.43
10:J:88:HIS:O	10:J:91:SER:OG	2.35	0.43
15:O:71:LEU:O	15:O:72:ARG:NH1	2.40	0.43
23:W:11:ARG:HE	23:W:15:GLU:HB2	1.83	0.43
40:p:15:ASP:N	40:p:15:ASP:OD1	2.48	0.43
48:x:17:ARG:HA	48:x:17:ARG:HD3	1.80	0.43
48:x:36:ARG:HA	48:x:47:THR:HA	1.99	0.43
51:1:45:G:H5''	51:1:46:G:C5'	2.36	0.43
51:1:121:G:H4'	51:1:149:A:H5'	1.99	0.43
51:1:227:A:H1'	51:1:229:C:N4	2.33	0.43
51:1:598:U:H2'	51:1:599:A:H8	1.83	0.43
51:1:1292:G:H2'	51:1:1293:C:C6	2.53	0.43
51:1:1960:A:H2'	51:1:1961:C:C5'	2.47	0.43
51:1:2326:C:H4'	51:1:2327:A:OP1	2.18	0.43
53:3:819:A:H5'	53:3:820:U:C5	2.53	0.43
53:3:1235:U:H2'	53:3:1236:A:O4'	2.18	0.43
58:B1:76:LYS:NZ	58:B1:76:LYS:HB3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:B2:300:ASP:OD1	59:B2:313:ALA:N	2.51	0.43
59:B2:515:MET:HE2	59:B2:515:MET:HB3	1.82	0.43
59:B2:1157:GLN:HG3	59:B2:1159:VAL:HG13	2.00	0.43
65:O:309:ARG:NH1	65:O:315:GLU:OE1	2.50	0.43
2:B:27:LEU:HD23	2:B:27:LEU:HA	1.74	0.43
7:G:15:PHE:HA	7:G:42:LEU:HD11	1.99	0.43
7:G:19:THR:HB	7:G:20:ARG:H	1.61	0.43
8:H:110:LEU:HD22	8:H:145:ALA:HB2	1.99	0.43
16:P:121:ARG:HA	16:P:122:PRO:HD3	1.82	0.43
35:k:2:ILE:HG13	35:k:62:VAL:HG11	1.99	0.43
39:o:26:LEU:HD13	39:o:39:VAL:HG22	2.00	0.43
43:s:77:ASP:OD1	43:s:77:ASP:N	2.48	0.43
47:w:33:ILE:HD11	47:w:78:ILE:HD11	2.00	0.43
51:1:196:A:N3	51:1:196:A:H2'	2.33	0.43
51:1:566:U:O2'	51:1:567:U:H5'	2.18	0.43
51:1:596:U:H2'	51:1:597:G:H8	1.84	0.43
51:1:784:G:OP1	51:1:2588:G:H5''	2.18	0.43
51:1:816:C:H2'	51:1:817:C:C6	2.53	0.43
51:1:1056:G:H21	51:1:1102:C:H5	1.65	0.43
51:1:2250:G:N2	51:1:2496:C:H5''	2.33	0.43
51:1:2888:C:H2'	51:1:2889:C:H6	1.82	0.43
53:3:201:G:H21	53:3:469:C:H1'	1.82	0.43
53:3:650:G:O2'	53:3:651:C:H5'	2.17	0.43
58:B1:211:GLU:CG	58:B1:215:LYS:HE3	2.44	0.43
58:B1:978:ARG:HD3	58:B1:999:TYR:H	1.83	0.43
58:B1:1079:LYS:HD3	58:B1:1098:GLN:HB3	1.99	0.43
62:5:63:G:H2'	62:5:64:A:C8	2.53	0.43
4:D:43:THR:HG23	4:D:44:VAL:H	1.84	0.43
7:G:170:ILE:HA	7:G:173:LYS:HE2	1.99	0.43
16:P:108:ASN:HB3	26:Z:6:ARG:HD3	1.99	0.43
22:V:15:LYS:CB	53:3:275:G:H5'	2.48	0.43
24:X:4:LEU:HD23	24:X:9:PHE:HB2	2.01	0.43
25:Y:34:VAL:HG11	25:Y:78:LEU:HD13	2.00	0.43
37:m:19:GLY:O	37:m:38:ARG:NH1	2.44	0.43
39:o:26:LEU:N	39:o:91:SER:O	2.48	0.43
40:p:74:GLN:HB2	40:p:77:SER:HB3	2.00	0.43
42:r:102:SER:OG	42:r:103:ALA:N	2.51	0.43
51:1:1156:A:H5'	51:1:1156:A:H8	1.83	0.43
51:1:1440:U:H2'	51:1:1441:G:C8	2.53	0.43
51:1:1808:A:H3'	51:1:1809:A:H8	1.82	0.43
53:3:273:U:H2'	53:3:274:A:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1517:G:O2'	53:3:1518:A:H5'	2.19	0.43
54:4:4:U:H2'	54:4:5:U:C6	2.53	0.43
56:9:33:DA:C5'	58:B1:121:PRO:HG3	2.36	0.43
58:B1:824:PRO:HD3	58:B1:835:LEU:HD12	2.00	0.43
58:B1:926:PRO:HB2	58:B1:1241:TYR:HE1	1.82	0.43
58:B1:1026:PRO:HB2	58:B1:1028:ILE:HG23	2.00	0.43
59:B2:811:ASN:ND2	59:B2:1098:LEU:O	2.51	0.43
12:L:86:VAL:HG12	12:L:150:PHE:CZ	2.53	0.43
16:P:24:ALA:HB2	16:P:29:THR:HG23	2.00	0.43
25:Y:25:SER:OG	53:3:1458:G:H5''	2.18	0.43
28:c:53:GLY:HA3	28:c:77:ARG:HG2	2.01	0.43
31:f:71:LEU:HD23	31:f:71:LEU:HA	1.84	0.43
40:p:52:ARG:HH21	51:1:2846:G:H5'	1.83	0.43
49:y:30:MET:SD	49:y:30:MET:N	2.91	0.43
51:1:532:A:H2'	51:1:532:A:N3	2.33	0.43
51:1:752:A:O2'	51:1:1781:U:H5'	2.18	0.43
51:1:941:A:O2'	51:1:1190:G:H4'	2.18	0.43
51:1:1117:C:H2'	51:1:1118:C:C6	2.54	0.43
51:1:2427:C:C5'	51:1:2429:G:H5'	2.47	0.43
51:1:2529:G:H5''	51:1:2530:A:H5''	2.01	0.43
53:3:247:G:O2'	53:3:248:C:H5'	2.18	0.43
53:3:846:G:H2'	53:3:847:G:H8	1.83	0.43
58:B1:201:LEU:CB	58:B1:221:ILE:HD13	2.47	0.43
59:B2:998:LEU:HG	59:B2:1011:LEU:HB3	1.99	0.43
60:W0:58:LEU:HD12	60:W0:59:ILE:HG12	2.00	0.43
65:0:190:ALA:N	65:0:205:GLU:O	2.52	0.43
10:J:137:ARG:HH12	53:3:1078:U:H4'	1.83	0.43
12:L:65:LEU:O	12:L:69:ARG:HG3	2.18	0.43
19:S:70:HIS:HB3	53:3:974:A:H5'	2.00	0.43
29:d:57:LYS:HB2	51:1:797:G:OP2	2.19	0.43
33:i:14:ALA:HB2	33:i:54:ILE:HG13	2.01	0.43
36:l:112:LEU:HD13	36:l:131:ALA:HA	2.00	0.43
37:m:53:MET:HE1	37:m:103:TYR:HB3	1.99	0.43
44:t:7:LEU:HD22	44:t:46:ALA:HB2	1.99	0.43
44:t:34:VAL:HG21	44:t:43:ILE:HD11	1.99	0.43
45:u:6:ARG:HB2	51:1:85:G:OP2	2.19	0.43
51:1:285:G:O2'	51:1:286:U:H5'	2.18	0.43
51:1:1595:C:H2'	51:1:1596:A:H8	1.84	0.43
53:3:182:A:H2'	53:3:183:C:H5''	2.01	0.43
53:3:839:C:H2'	53:3:840:C:H6	1.83	0.43
53:3:1028:C:H3'	53:3:1029:U:C5'	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1352:C:H2'	53:3:1353:G:H8	1.83	0.43
58:B1:111:THR:HG21	58:B1:303:VAL:HB	2.00	0.43
65:0:360:PHE:HD1	65:0:360:PHE:HA	1.71	0.43
5:E:40:LYS:HD3	51:1:2419:U:OP2	2.18	0.43
9:I:115:GLN:HE22	53:3:406:G:H1'	1.84	0.43
14:N:40:ARG:HD2	14:N:40:ARG:HA	1.78	0.43
20:T:17:ASP:OD1	20:T:17:ASP:N	2.51	0.43
33:i:72:THR:HB	33:i:115:ASP:HB2	2.01	0.43
39:o:15:ARG:CZ	52:2:8:C:H5''	2.49	0.43
51:1:1417:C:H2'	51:1:1418:G:O4'	2.19	0.43
51:1:1726:C:H2'	51:1:1727:C:H6	1.82	0.43
51:1:2055:C:H5'	51:1:2056:G:O5'	2.18	0.43
51:1:2461:A:H1'	51:1:2492:U:N3	2.33	0.43
53:3:1261:A:H5''	53:3:1262:C:C5	2.53	0.43
58:B1:58:CYS:SG	58:B1:60:ARG:HG2	2.59	0.43
58:B1:111:THR:CG2	58:B1:300:GLN:HA	2.48	0.43
59:B2:444:ASP:OD1	59:B2:444:ASP:N	2.51	0.43
59:B2:829:THR:HG23	59:B2:1059:ARG:HG2	2.00	0.43
65:0:617:MET:N	65:0:658:VAL:O	2.47	0.43
5:E:4:LYS:O	36:l:48:ARG:NH1	2.43	0.43
5:E:56:LEU:HD22	36:l:49:GLY:HA2	2.00	0.43
7:G:55:GLU:HB2	7:G:183:PHE:HZ	1.84	0.43
18:R:47:LEU:HD22	18:R:51:GLN:HE21	1.83	0.43
28:c:164:GLN:HE22	51:1:2822:G:H5''	1.83	0.43
29:d:158:PHE:HA	29:d:169:VAL:HG21	2.00	0.43
32:g:5:LEU:HD22	32:g:9:VAL:HG21	2.01	0.43
33:i:27:LEU:HD11	33:i:34:ILE:HD13	2.00	0.43
41:q:30:VAL:HG13	51:1:580:U:O3'	2.19	0.43
47:w:62:LYS:HE3	47:w:81:GLU:HG3	2.00	0.43
51:1:1925:C:H2'	51:1:1926:U:O4'	2.18	0.43
51:1:1926:U:H2'	51:1:1927:A:H8	1.83	0.43
51:1:2086:U:H2'	51:1:2087:G:C8	2.53	0.43
51:1:2484:G:O2'	51:1:2485:G:H5'	2.19	0.43
53:3:556:C:O2'	53:3:557:G:H5'	2.19	0.43
53:3:1479:C:H2'	53:3:1480:A:C8	2.51	0.43
53:3:1517:G:C2'	53:3:1518:A:H5'	2.49	0.43
57:A1:68:TYR:HE1	57:A1:79:LEU:HD13	1.82	0.43
57:A1:211:ILE:HD12	57:A1:211:ILE:HA	1.92	0.43
58:B1:120:LEU:HD22	58:B1:120:LEU:HA	1.77	0.43
58:B1:141:PHE:HE2	58:B1:296:LYS:CB	2.23	0.43
58:B1:850:LYS:HB3	58:B1:855:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:894:VAL:HG22	58:B1:1258:ARG:HH11	1.83	0.43
3:C:20:TYR:OH	51:1:2348:U:H5'	2.19	0.43
7:G:163:ILE:HD11	7:G:213:LEU:HD21	2.01	0.43
10:J:12:GLU:HA	10:J:38:VAL:HG12	2.00	0.43
15:O:24:GLU:O	15:O:28:THR:OG1	2.34	0.43
19:S:58:ARG:HD2	53:3:980:C:H1'	2.01	0.43
22:V:24:ILE:HG23	22:V:41:THR:HB	1.99	0.43
27:b:7:PRO:HA	27:b:13:ARG:HA	1.99	0.43
30:e:48:LEU:O	30:e:52:ALA:N	2.50	0.43
33:i:134:SER:HB2	51:1:1077:A:C2	2.54	0.43
36:l:28:GLY:H	36:l:31:GLY:HA2	1.83	0.43
37:m:1:MET:SD	37:m:1:MET:N	2.88	0.43
37:m:109:PRO:HD2	37:m:112:LEU:HD11	2.00	0.43
51:1:69:C:O2'	51:1:70:G:H5'	2.18	0.43
51:1:1047:G:H2'	51:1:1110:G:N2	2.34	0.43
51:1:1063:G:H5''	51:1:1064:C:C5	2.53	0.43
51:1:1441:G:H4'	51:1:1628:G:C5'	2.49	0.43
51:1:2128:G:OP1	64:a:38:PHE:HB3	2.19	0.43
53:3:220:G:O2'	53:3:221:C:H5'	2.18	0.43
58:B1:568:SER:HB3	58:B1:570:LYS:NZ	2.34	0.43
59:B2:646:SER:OG	59:B2:647:ARG:N	2.52	0.43
64:a:189:LEU:O	64:a:193:LEU:N	2.44	0.43
65:0:245:GLU:HA	65:0:248:ILE:HD12	2.01	0.43
3:C:10:LEU:HD21	3:C:33:LEU:HD23	2.01	0.43
7:G:123:GLY:HA3	7:G:127:LYS:HE2	2.00	0.43
8:H:172:VAL:HG23	53:3:1107:C:H5''	2.00	0.43
18:R:107:THR:HG21	53:3:1306:A:N3	2.33	0.43
24:X:43:MET:HE2	24:X:43:MET:HB2	1.92	0.43
29:d:110:SER:O	29:d:114:ARG:NE	2.52	0.43
50:z:10:ARG:NH1	51:1:1000:A:O2'	2.52	0.43
51:1:466:A:H2'	51:1:467:G:H5'	2.01	0.43
51:1:1837:C:H2'	51:1:1899:A:N6	2.32	0.43
51:1:2724:U:H2'	51:1:2725:A:C8	2.54	0.43
53:3:52:C:H2'	53:3:53:A:C8	2.54	0.43
58:B1:388:ARG:HG2	58:B1:388:ARG:HH11	1.84	0.43
58:B1:515:ARG:HH12	58:B1:724:MET:HG2	1.84	0.43
59:B2:22:LEU:HB3	59:B2:655:VAL:HG11	2.01	0.43
65:0:505:HIS:N	65:0:516:GLY:O	2.43	0.43
65:0:520:ILE:HB	65:0:576:ILE:HD11	1.99	0.43
4:D:25:LYS:HE2	4:D:25:LYS:HB2	1.89	0.43
8:H:19:SER:OG	19:S:91:GLU:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:86:VAL:HG12	12:L:150:PHE:CE2	2.53	0.43
16:P:34:THR:HA	16:P:40:ALA:HA	2.00	0.43
25:Y:54:GLN:HE21	53:3:193:C:H1'	1.83	0.43
28:c:118:PHE:HE1	51:1:2048:G:H21	1.66	0.43
32:g:55:GLU:O	32:g:59:ALA:N	2.50	0.43
51:1:792:A:H3'	51:1:793:A:H5'	2.00	0.43
51:1:919:U:H2'	51:1:920:A:O4'	2.19	0.43
51:1:1091:G:O6	51:1:1099:G:O6	2.36	0.43
51:1:1289:C:O2'	51:1:1330:C:H4'	2.19	0.43
51:1:1343:G:N3	51:1:1343:G:H2'	2.33	0.43
51:1:1557:C:C5	51:1:1558:C:H2'	2.54	0.43
51:1:1923:U:H2'	51:1:1924:C:C6	2.54	0.43
51:1:2122:U:H2'	51:1:2123:G:O4'	2.18	0.43
51:1:2170:A:C4	51:1:2171:A:H8	2.37	0.43
51:1:2340:A:H2'	51:1:2341:G:H8	1.84	0.43
53:3:605:U:O2'	53:3:606:G:H5'	2.19	0.43
53:3:613:C:H2'	53:3:614:C:C6	2.53	0.43
58:B1:62:PHE:N	58:B1:62:PHE:CD1	2.86	0.43
58:B1:96:LYS:NZ	59:B2:1298:VAL:HG11	2.34	0.43
58:B1:434:ILE:HD11	59:B2:1274:GLU:CG	2.49	0.43
58:B1:559:ALA:HB3	58:B1:562:GLU:HB3	2.01	0.43
62:5:25:C:H2'	62:5:26:A:H8	1.84	0.43
64:a:47:ASN:HD22	64:a:170:ILE:HG13	1.84	0.43
64:a:51:ASP:HB3	64:a:54:LYS:HB3	2.01	0.43
64:a:216:THR:HG22	64:a:217:THR:H	1.83	0.43
8:H:113:LYS:HB2	8:H:184:ASN:HD22	1.84	0.42
9:I:23:GLY:HA3	53:3:409:U:OP1	2.19	0.42
10:J:111:ARG:O	10:J:115:GLU:N	2.51	0.42
13:M:91:LEU:HD23	13:M:91:LEU:HA	1.86	0.42
20:T:70:LYS:HE3	20:T:70:LYS:HB2	1.88	0.42
27:b:186:ASP:OD1	32:g:123:ARG:NH2	2.52	0.42
37:m:64:TRP:NE1	51:1:873:C:H4'	2.33	0.42
51:1:20:C:H2'	51:1:21:A:C8	2.53	0.42
53:3:865:A:H5'	53:3:1078:U:O4	2.18	0.42
55:8:1:DC:H5''	58:B1:210:SER:HG	1.80	0.42
58:B1:24:LEU:HD21	58:B1:116:PHE:CE2	2.54	0.42
58:B1:128:LEU:CD2	58:B1:188:LEU:HB3	2.47	0.42
58:B1:375:GLU:HB3	59:B2:1245:ALA:CB	2.48	0.42
59:B2:125:GLY:H	59:B2:495:ALA:HB1	1.84	0.42
59:B2:538:LEU:HD13	59:B2:543:ALA:HB2	2.00	0.42
4:D:21:ARG:NH2	51:1:684:G:OP1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:134:LEU:O	7:G:137:THR:OG1	2.37	0.42
14:N:51:LEU:HD13	14:N:56:MET:HG3	2.02	0.42
18:R:6:ILE:HG13	18:R:7:ASN:H	1.84	0.42
21:U:13:LYS:HE2	53:3:392:C:H5'	2.01	0.42
21:U:21:VAL:HG12	21:U:33:ILE:HB	2.01	0.42
41:q:24:TYR:CE1	51:1:17:G:H4'	2.54	0.42
51:1:526:A:N6	51:1:2626:C:H4'	2.35	0.42
51:1:1132:U:H2'	51:1:1133:A:C8	2.55	0.42
51:1:1786:A:H1'	51:1:1938:A:N6	2.34	0.42
53:3:1211:U:H4'	53:3:1213:A:N3	2.35	0.42
54:4:43:G:H5'	59:B2:688:GLN:HE22	1.84	0.42
59:B2:469:VAL:HA	59:B2:472:GLU:HG2	2.02	0.42
59:B2:616:ILE:HG13	59:B2:652:TYR:HB2	2.01	0.42
59:B2:741:MET:HE3	59:B2:974:ARG:HH12	1.84	0.42
5:E:54:LEU:HD12	5:E:54:LEU:HA	1.91	0.42
9:I:27:ILE:H	9:I:27:ILE:HG13	1.73	0.42
10:J:137:ARG:NH1	53:3:1078:U:H4'	2.34	0.42
10:J:146:MET:HE2	10:J:146:MET:HB3	1.90	0.42
14:N:17:ARG:HH12	53:3:1129:C:H5'	1.84	0.42
17:Q:86:VAL:HG22	17:Q:95:HIS:CE1	2.54	0.42
19:S:81:ILE:HG21	53:3:1202:U:C2	2.55	0.42
21:U:20:VAL:HG12	21:U:35:ARG:HA	2.01	0.42
28:c:12:THR:OG1	28:c:13:ARG:N	2.51	0.42
31:f:70:LEU:HD11	51:1:2758:A:N1	2.34	0.42
36:l:19:LEU:HD23	51:1:587:C:O2	2.18	0.42
37:m:57:VAL:HB	37:m:60:GLN:HB3	2.01	0.42
37:m:112:LEU:HA	37:m:115:GLU:HB3	2.00	0.42
51:1:186:G:O2'	51:1:187:G:H5'	2.19	0.42
51:1:288:U:H2'	51:1:289:G:H8	1.83	0.42
51:1:1536:C:H4'	51:1:1537:G:C2	2.54	0.42
51:1:2323:G:O2'	51:1:2324:U:H5'	2.19	0.42
51:1:2720:U:H5'	51:1:2720:U:C6	2.53	0.42
51:1:2881:U:H2'	51:1:2882:A:H8	1.83	0.42
53:3:879:C:H2'	53:3:880:C:C6	2.54	0.42
53:3:1062:U:H2'	53:3:1063:C:C6	2.54	0.42
57:A1:48:LEU:HD12	57:A1:48:LEU:HA	1.78	0.42
57:A1:76:GLU:HB3	57:A1:80:GLU:HB3	2.01	0.42
58:B1:201:LEU:HD23	58:B1:201:LEU:HA	1.92	0.42
58:B1:242:LEU:C	58:B1:242:LEU:HD23	2.44	0.42
58:B1:385:LEU:CD2	58:B1:390:LEU:HB2	2.50	0.42
58:B1:515:ARG:NH2	58:B1:718:SER:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:820:ILE:HG12	58:B1:884:SER:HB2	2.01	0.42
58:B1:950:ILE:HB	58:B1:1018:ALA:HB3	2.01	0.42
59:B2:590:PRO:HB2	59:B2:655:VAL:HG21	2.01	0.42
63:6:17(A):U:O2'	63:6:18:G:H5''	2.19	0.42
5:E:27:ASN:O	5:E:35:LYS:NZ	2.47	0.42
10:J:75:LEU:H	10:J:75:LEU:HG	1.40	0.42
14:N:122:ARG:HG3	53:3:1343:G:O2'	2.18	0.42
18:R:111:PRO:HB2	18:R:113:LYS:HG3	2.02	0.42
22:V:30:HIS:HD2	22:V:33:TYR:H	1.66	0.42
27:b:200:MET:HG3	51:1:1820:U:C2	2.54	0.42
31:f:136:ASP:HB3	31:f:139:VAL:HG22	2.00	0.42
32:g:116:ARG:HA	32:g:116:ARG:HD3	1.82	0.42
35:k:22:ILE:HD12	51:1:1952:A:C2	2.55	0.42
36:l:78:ARG:CZ	51:1:626:A:H2'	2.49	0.42
43:s:28:LYS:O	43:s:32:ALA:N	2.50	0.42
51:1:467:G:O2'	51:1:468:G:H5'	2.20	0.42
51:1:1278:C:H2'	51:1:1279:G:C8	2.54	0.42
53:3:794:A:H4'	53:3:1521:C:O2'	2.19	0.42
53:3:1330:U:H2'	53:3:1331:G:O4'	2.19	0.42
58:B1:144:TYR:CE1	58:B1:162:GLU:OE1	2.73	0.42
58:B1:362:ARG:HB2	58:B1:364:HIS:HD2	1.83	0.42
59:B2:50:GLU:HG2	59:B2:73:TYR:HE1	1.85	0.42
59:B2:524:ILE:HD12	59:B2:712:SER:HB2	2.02	0.42
65:0:70:ALA:N	65:0:84:ILE:O	2.48	0.42
65:0:170:GLN:NE2	65:0:266:CYS:H	2.18	0.42
12:L:115:MET:HB3	53:3:1240:U:OP2	2.20	0.42
14:N:17:ARG:HH12	53:3:1129:C:H4'	1.85	0.42
17:Q:29:LYS:HA	17:Q:29:LYS:HD2	1.79	0.42
19:S:50:LEU:HD23	19:S:50:LEU:HA	1.85	0.42
20:T:80:LEU:HD12	20:T:80:LEU:HA	1.90	0.42
28:c:35:THR:OG1	28:c:49:GLN:O	2.36	0.42
28:c:148:GLN:HB2	28:c:152:PRO:HG3	2.01	0.42
30:e:84:ILE:HG21	51:1:2312:U:C4'	2.48	0.42
33:i:67:THR:HG22	33:i:68:PHE:H	1.84	0.42
33:i:133:ARG:HD2	33:i:133:ARG:HA	1.82	0.42
34:j:60:ASP:HA	34:j:93:ILE:HD11	2.00	0.42
41:q:73:ILE:HD11	41:q:77:LYS:HB3	2.01	0.42
51:1:1539:U:H2'	51:1:1540:G:H8	1.83	0.42
51:1:2233:U:H2'	51:1:2234:G:C8	2.54	0.42
51:1:2425:A:H4'	51:1:2426:A:C5'	2.49	0.42
51:1:2743:U:H2'	51:1:2744:G:C4'	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1065:U:P	53:3:1190:G:H22	2.42	0.42
58:B1:141:PHE:CD2	58:B1:297:ARG:HB2	2.54	0.42
58:B1:245:LEU:CG	58:B1:246:PRO:HD2	2.47	0.42
58:B1:390:LEU:N	58:B1:390:LEU:HD13	2.35	0.42
58:B1:797:THR:HG22	58:B1:924:GLY:HA3	2.01	0.42
58:B1:1350:ASN:HA	58:B1:1353:VAL:HG12	2.02	0.42
59:B2:6:THR:OG1	59:B2:781:ASP:OD1	2.33	0.42
59:B2:559:CYS:HA	59:B2:560:PRO:HD3	1.90	0.42
59:B2:1275:VAL:HG13	59:B2:1287:LEU:HD11	2.00	0.42
62:5:4:C:H2'	62:5:5:G:C8	2.55	0.42
13:M:31:LEU:HD22	53:3:643:C:H5''	2.01	0.42
18:R:96:VAL:HG22	53:3:1308:U:OP1	2.20	0.42
34:j:104:ALA:CB	51:1:1139:G:H5'	2.49	0.42
36:l:51:GLU:OE1	36:l:60:ARG:NH1	2.52	0.42
40:p:2:ASN:ND2	51:1:2876:G:H4'	2.32	0.42
44:t:38:ALA:O	44:t:81:LYS:NZ	2.39	0.42
51:1:970:U:H2'	51:1:971:G:C8	2.55	0.42
51:1:1071:G:H5''	51:1:1072:C:H5	1.84	0.42
51:1:1916:A:N1	53:3:1409:C:H5'	2.34	0.42
51:1:1922:G:H2'	51:1:1923:U:O4'	2.19	0.42
51:1:2039:U:H2'	51:1:2040:G:C8	2.55	0.42
51:1:2534:A:H2'	51:1:2535:G:H5''	2.02	0.42
51:1:2788:C:H2'	51:1:2789:C:C6	2.53	0.42
53:3:66:A:H5'	53:3:173:U:C4	2.55	0.42
53:3:146:G:O2'	53:3:147:G:H5'	2.20	0.42
57:A2:28:LEU:HB2	57:A2:201:LEU:HB3	2.02	0.42
58:B1:59:ALA:HB1	58:B1:90:VAL:HG23	2.01	0.42
58:B1:647:PRO:HG3	58:B1:697:MET:HB3	2.01	0.42
58:B1:1289:ASN:O	58:B1:1293:GLU:HB2	2.20	0.42
59:B2:699:LEU:HG	59:B2:799:ASN:HD22	1.85	0.42
65:0:148:GLY:N	65:0:176:GLU:OE1	2.52	0.42
65:0:504:LYS:HE2	65:0:504:LYS:HB2	1.82	0.42
65:0:505:HIS:CE1	65:0:595:LEU:HB3	2.55	0.42
3:C:35:LEU:HD13	3:C:37:LYS:HE2	2.01	0.42
6:F:18:LYS:HE2	6:F:18:LYS:HB3	1.83	0.42
15:O:47:GLU:HG3	53:3:1254:A:OP1	2.19	0.42
36:l:2:ARG:NH1	36:l:5:THR:HG1	2.18	0.42
36:l:90:VAL:N	36:l:121:THR:O	2.52	0.42
46:v:42:LEU:HD12	46:v:47:VAL:HG11	2.02	0.42
48:x:22:ASN:HD22	48:x:22:ASN:HA	1.65	0.42
51:1:198:C:O5'	51:1:198:C:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1545:A:H2'	51:1:1546:G:O4'	2.19	0.42
51:1:2314:A:H2'	51:1:2315:G:C8	2.54	0.42
51:1:2533:U:H2'	51:1:2534:A:O4'	2.19	0.42
53:3:97:G:H2'	53:3:98:A:O4'	2.20	0.42
53:3:505:G:O5'	53:3:505:G:H8	2.02	0.42
53:3:521:G:O2'	53:3:522:C:H5'	2.19	0.42
53:3:1341:U:O2'	53:3:1342:C:H5'	2.20	0.42
58:B1:137:ARG:HA	58:B1:142:GLU:HG2	2.01	0.42
8:H:122:GLN:NE2	8:H:127:VAL:HG21	2.34	0.42
14:N:95:SER:OG	14:N:96:GLU:N	2.53	0.42
18:R:7:ASN:HD21	18:R:18:LEU:HD13	1.84	0.42
19:S:30:ILE:H	19:S:30:ILE:HG13	1.62	0.42
27:b:167:ASP:OD2	53:3:682:G:H5'	2.19	0.42
28:c:123:LYS:HE2	38:n:1:MET:HE1	2.01	0.42
30:e:176:PHE:HD1	30:e:176:PHE:HA	1.76	0.42
32:g:11:ASN:ND2	51:1:2095:A:O5'	2.53	0.42
32:g:118:PRO:HD2	32:g:130:VAL:HG13	2.01	0.42
51:1:239:C:H2'	51:1:240:C:O4'	2.20	0.42
51:1:744:U:H4'	51:1:1658:C:H4'	2.01	0.42
51:1:1201:U:H2'	51:1:1202:G:C8	2.54	0.42
51:1:1278:C:H2'	51:1:1279:G:H8	1.85	0.42
51:1:2240:U:H2'	51:1:2241:A:H8	1.85	0.42
51:1:2332:C:H2'	51:1:2335:A:C2	2.55	0.42
51:1:2685:G:H2'	51:1:2686:G:H8	1.84	0.42
51:1:2736:A:H2'	51:1:2737:G:H8	1.85	0.42
53:3:1163:A:H2'	53:3:1164:G:C8	2.55	0.42
53:3:1306:A:H2'	53:3:1307:U:O4'	2.20	0.42
53:3:1494:G:H8	53:3:1494:G:OP2	2.03	0.42
65:0:16:SER:OG	65:0:89:THR:OG1	2.26	0.42
7:G:66:ILE:HB	7:G:88:GLN:HG3	2.02	0.42
9:I:40:HIS:HB3	9:I:43:ARG:HH21	1.85	0.42
17:Q:88:ASP:HB3	53:3:523:A:H61	1.84	0.42
25:Y:43:LYS:HE2	25:Y:43:LYS:HB2	1.91	0.42
27:b:143:VAL:HB	27:b:153:LEU:HD22	2.01	0.42
33:i:131:THR:HG22	33:i:135:MET:CE	2.50	0.42
36:l:55:MET:HA	36:l:56:PRO:HD3	1.88	0.42
41:q:84:LYS:HB3	41:q:115:ALA:HB1	2.02	0.42
50:z:13:ILE:H	50:z:13:ILE:HG13	1.69	0.42
51:1:123:G:H5''	51:1:1375:U:O2'	2.20	0.42
51:1:436:C:H2'	51:1:437:U:C6	2.55	0.42
51:1:627:A:H8	51:1:627:A:OP1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1068:G:H21	51:1:1096:A:H5'	1.85	0.42
51:1:1069:A:H2	51:1:1096:A:OP1	2.02	0.42
51:1:1494:A:H2'	51:1:1495:A:O4'	2.20	0.42
51:1:1649:G:H2'	51:1:1650:A:H8	1.84	0.42
51:1:2138:G:C2'	51:1:2139:U:H5'	2.49	0.42
51:1:2480:C:OP2	51:1:2537:U:H4'	2.20	0.42
53:3:34:C:H2'	53:3:35:G:C8	2.54	0.42
53:3:749:A:H2'	53:3:750:C:O4'	2.20	0.42
53:3:768:A:H2'	53:3:769:G:O4'	2.20	0.42
53:3:1049:U:H4'	53:3:1050:G:H5''	2.02	0.42
58:B1:220:ARG:HH11	58:B1:220:ARG:CG	2.26	0.42
63:6:69:C:H2'	63:6:70:G:C5'	2.39	0.42
65:0:487:GLN:HB3	65:0:488:VAL:H	1.70	0.42
1:A:37:CYS:H	1:A:40:CYS:HB3	1.85	0.42
7:G:70:GLY:HA3	7:G:163:ILE:HB	2.02	0.42
22:V:70:LYS:HD3	53:3:254:G:H5''	2.02	0.42
25:Y:56:ILE:HD13	25:Y:59:ARG:HH22	1.84	0.42
27:b:258:SER:O	27:b:258:SER:OG	2.34	0.42
29:d:130:LYS:HA	51:1:321:U:OP2	2.19	0.42
34:j:27:ARG:HD2	51:1:1143:A:N6	2.35	0.42
34:j:44:TYR:O	41:q:63:ARG:NE	2.53	0.42
38:n:64:ARG:NH2	51:1:2852:G:H5'	2.34	0.42
47:w:58:LYS:HE2	51:1:2366:A:H4'	2.01	0.42
51:1:1120:G:H2'	51:1:1121:C:O4'	2.20	0.42
51:1:1258:U:H2'	51:1:1259:G:H8	1.85	0.42
51:1:1449:G:O2'	51:1:1450:G:H5'	2.20	0.42
51:1:2432:A:H1'	63:6:75:C:O4'	2.20	0.42
51:1:2689:U:O2	51:1:2713:U:H5''	2.19	0.42
51:1:2704:C:H2'	51:1:2705:A:O4'	2.20	0.42
53:3:1223:C:C5	53:3:1224:U:H5	2.38	0.42
58:B1:102:MET:HG2	58:B1:246:PRO:CG	2.49	0.42
58:B1:222:LYS:HA	58:B1:222:LYS:HD2	1.33	0.42
58:B1:513:MET:HG3	58:B1:544:LEU:HD11	2.01	0.42
58:B1:586:GLY:HA3	58:B1:612:LEU:HD11	2.01	0.42
59:B2:487:LEU:HA	59:B2:487:LEU:HD22	1.77	0.42
62:5:17:C:H6	62:5:17:C:H2'	1.69	0.42
5:E:15:LYS:HB2	5:E:64:ALA:HB1	2.02	0.41
12:L:114:SER:OG	12:L:115:MET:N	2.53	0.41
16:P:118:ASN:HB2	53:3:718:A:H5'	2.02	0.41
25:Y:55:PRO:HA	53:3:194:C:H5'	2.02	0.41
27:b:110:LYS:N	27:b:113:ASP:OD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:253:GLY:HA2	51:1:1797:G:H5'	2.01	0.41
34:j:125:TYR:OH	34:j:132:HIS:NE2	2.45	0.41
41:q:23:TYR:CE1	51:1:533:G:H5'	2.55	0.41
47:w:14:ALA:HB1	51:1:2271:G:OP1	2.20	0.41
51:1:479:A:H1'	51:1:481:G:H5''	2.02	0.41
51:1:1275:A:N6	51:1:1296:G:H4'	2.35	0.41
51:1:2547:A:H2'	51:1:2548:U:C6	2.55	0.41
51:1:2773:C:H2'	51:1:2774:C:H6	1.85	0.41
53:3:834:U:H2'	53:3:835:U:C6	2.55	0.41
53:3:1428:A:OP2	53:3:1428:A:O4'	2.37	0.41
58:B1:243:PRO:HG2	59:B2:1332:SER:C	2.44	0.41
58:B1:244:VAL:HA	58:B1:269:TYR:OH	2.19	0.41
65:0:34:THR:OG1	65:0:71:PHE:O	2.37	0.41
65:0:665:GLY:O	65:0:668:THR:OG1	2.37	0.41
9:I:66:VAL:HB	9:I:71:PHE:HD2	1.84	0.41
21:U:6:LEU:HD11	21:U:70:ARG:HD2	2.01	0.41
36:l:57:LEU:HD12	36:l:57:LEU:HA	1.93	0.41
41:q:90:ASP:OD2	51:1:996:A:H4'	2.19	0.41
51:1:181:A:H2'	51:1:182:A:C8	2.55	0.41
51:1:234:U:O2'	51:1:235:U:H5'	2.19	0.41
51:1:278:A:H2'	51:1:278:A:N3	2.34	0.41
51:1:2259:U:H2'	51:1:2260:C:H6	1.85	0.41
51:1:2361:G:O2'	51:1:2362:C:H5'	2.20	0.41
51:1:2698:U:H2'	51:1:2699:C:C6	2.55	0.41
53:3:114:U:O2'	53:3:115:G:H5'	2.20	0.41
57:A2:48:LEU:HA	57:A2:48:LEU:HD23	1.86	0.41
58:B1:224:LEU:HD23	58:B1:224:LEU:HA	1.89	0.41
58:B1:596:LEU:HD23	58:B1:596:LEU:HA	1.91	0.41
58:B1:609:TYR:HD2	58:B1:610:ARG:NH1	2.17	0.41
58:B1:616:PRO:HA	58:B1:619:ILE:HG22	2.02	0.41
58:B1:848:VAL:HB	58:B1:858:VAL:HG22	2.02	0.41
58:B1:1024:THR:HG23	58:B1:1123:ARG:HA	2.00	0.41
59:B2:1244:HIS:NE2	59:B2:1266:GLY:O	2.44	0.41
65:0:210:ASP:OD1	65:0:210:ASP:N	2.52	0.41
8:H:156:LEU:H	8:H:156:LEU:HG	1.67	0.41
28:c:149:ASN:HB2	51:1:2574:G:O2'	2.20	0.41
30:e:133:GLU:HG3	30:e:135:ILE:H	1.84	0.41
34:j:108:MET:HB3	51:1:1006:C:O2'	2.20	0.41
36:l:59:ARG:HD2	51:1:250:G:H4'	2.03	0.41
37:m:88:ASN:OD1	37:m:88:ASN:N	2.52	0.41
47:w:18:GLY:N	47:w:35:ARG:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:353:C:H2'	51:1:354:A:H8	1.85	0.41
51:1:524:G:H5'	51:1:539:G:N2	2.35	0.41
51:1:596:U:H2'	51:1:597:G:C8	2.55	0.41
51:1:1062:G:O2'	51:1:1063:G:C4'	2.69	0.41
51:1:1917:U:O2'	51:1:1918:A:H5'	2.20	0.41
53:3:1037:C:H2'	53:3:1038:C:C6	2.54	0.41
53:3:1129:C:H42	53:3:1143:G:H1	1.66	0.41
53:3:1311:A:H2'	53:3:1312:G:O4'	2.20	0.41
55:8:3:DC:N1	55:8:4:DT:H72	2.34	0.41
58:B1:515:ARG:HG2	58:B1:516:ASP:H	1.85	0.41
59:B2:478:ARG:HD2	59:B2:492:MET:HA	2.02	0.41
65:0:69:THR:OG1	65:0:367:HIS:NE2	2.34	0.41
11:K:9:MET:HE3	11:K:86:ARG:HB3	2.03	0.41
11:K:45:ARG:HA	11:K:45:ARG:HD3	1.87	0.41
18:R:106:ARG:HB3	53:3:947:G:OP1	2.20	0.41
23:W:11:ARG:NH2	53:3:845:A:H4'	2.36	0.41
23:W:11:ARG:NH1	53:3:845:A:H5'	2.35	0.41
27:b:209:ALA:HA	27:b:212:TRP:CE2	2.55	0.41
28:c:130:GLN:HE22	51:1:2578:G:H21	1.69	0.41
36:l:95:LEU:HD22	36:l:100:ILE:HD11	2.01	0.41
49:y:41:HIS:CD2	51:1:96:C:H4'	2.55	0.41
51:1:690:G:H2'	51:1:691:C:O4'	2.19	0.41
51:1:1318:U:H2'	51:1:1319:C:H6	1.83	0.41
51:1:1645:G:C5'	51:1:1646:C:H5'	2.31	0.41
51:1:1882:U:H2'	51:1:1883:U:C6	2.54	0.41
51:1:2701:U:H3'	51:1:2702:G:H5''	2.02	0.41
51:1:2802:G:H2'	51:1:2803:G:O4'	2.20	0.41
51:1:2834:G:H2'	51:1:2879:A:H61	1.84	0.41
52:2:78:A:H2'	52:2:79:G:O4'	2.19	0.41
53:3:216:U:H2'	53:3:217:C:C6	2.55	0.41
53:3:226:G:O2'	53:3:227:G:H5'	2.21	0.41
53:3:675:A:H2'	53:3:676:A:O4'	2.19	0.41
53:3:947:G:H4'	53:3:1332:A:H2	1.86	0.41
53:3:1499:A:O2'	53:3:1520:C:H5'	2.19	0.41
5:E:33:THR:C	5:E:35:LYS:H	2.28	0.41
6:F:1:MET:HE2	6:F:1:MET:HB2	1.89	0.41
8:H:5:HIS:HA	8:H:6:PRO:HD3	1.94	0.41
8:H:126:ARG:HD3	8:H:126:ARG:HA	1.67	0.41
9:I:24:VAL:H	53:3:409:U:C5'	2.33	0.41
13:M:12:ARG:HD2	13:M:26:MET:HE2	2.02	0.41
17:Q:101:LEU:O	17:Q:103:CYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:13:HIS:CE1	53:3:1296:C:H5'	2.56	0.41
19:S:97:LYS:HE2	19:S:97:LYS:HB3	1.86	0.41
32:g:14:SER:O	32:g:14:SER:OG	2.36	0.41
32:g:43:ASN:O	32:g:47:PHE:N	2.54	0.41
35:k:17:ARG:NH1	53:3:1471:U:OP1	2.53	0.41
51:1:373:U:H2'	51:1:374:A:H8	1.85	0.41
51:1:974:G:N3	51:1:974:G:H2'	2.35	0.41
51:1:1017:G:C6	51:1:1018:U:O4	2.73	0.41
51:1:2096:C:H2'	51:1:2097:A:C8	2.55	0.41
51:1:2385:C:H2'	51:1:2386:A:H8	1.86	0.41
51:1:2564:A:OP1	51:1:2648:G:H4'	2.21	0.41
51:1:2692:G:H1'	51:1:2847:U:H1'	2.02	0.41
53:3:244:U:O4	53:3:906:A:H1'	2.20	0.41
53:3:987:G:H2'	53:3:988:G:C8	2.55	0.41
58:B1:109:SER:CB	58:B1:296:LYS:HG2	2.51	0.41
58:B1:144:TYR:CD1	58:B1:144:TYR:N	2.88	0.41
58:B1:279:LEU:HD13	58:B1:299:LEU:HD13	2.02	0.41
59:B2:1313:HIS:CD2	60:W0:31:GLN:HE22	2.37	0.41
15:O:61:ALA:HB2	53:3:1061:G:H5''	2.03	0.41
16:P:38:GLY:HA2	53:3:708:C:O4'	2.19	0.41
19:S:86:ALA:HB1	19:S:91:GLU:HB2	2.03	0.41
33:i:94:LYS:NZ	51:1:1076:C:H4'	2.36	0.41
36:l:99:ASN:ND2	51:1:621:A:OP2	2.54	0.41
44:t:23:ALA:HB1	44:t:29:THR:HB	2.02	0.41
50:z:10:ARG:HB2	50:z:53:MET:CB	2.50	0.41
51:1:799:G:H5''	51:1:800:A:H2'	2.02	0.41
51:1:1019:U:OP1	51:1:1036:G:C5'	2.45	0.41
51:1:1872:A:H2'	51:1:1873:G:H5'	2.02	0.41
51:1:2427:C:H5''	51:1:2429:G:H5'	2.02	0.41
53:3:47:C:H4'	53:3:48:C:O5'	2.21	0.41
53:3:627:G:H2'	53:3:628:G:O4'	2.21	0.41
53:3:817:C:H4'	53:3:818:G:H5''	2.03	0.41
53:3:842:U:H2'	53:3:844:G:H5'	2.02	0.41
53:3:938:A:H1'	53:3:1376:U:O2'	2.21	0.41
57:A1:205:MET:HE1	57:A1:217:ILE:HG13	2.03	0.41
58:B1:839:VAL:HG12	58:B1:864:LEU:HD12	2.02	0.41
58:B1:930:LEU:HA	58:B1:1244:GLN:HG3	2.02	0.41
58:B1:1177:ILE:HD12	58:B1:1186:TYR:HE2	1.85	0.41
59:B2:998:LEU:HD21	59:B2:1015:ALA:HB2	2.02	0.41
65:0:513:GLY:O	65:0:584:HIS:CD2	2.74	0.41
9:I:205:LYS:NZ	53:3:26:A:H2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:7:ASN:O	18:R:9:PRO:HD3	2.20	0.41
22:V:9:GLY:H	22:V:24:ILE:HD13	1.86	0.41
22:V:57:VAL:HG13	22:V:78:VAL:HB	2.03	0.41
27:b:55:GLY:HA2	51:1:692:C:OP1	2.21	0.41
29:d:79:ARG:HE	29:d:79:ARG:HB2	1.76	0.41
33:i:92:PRO:CB	51:1:1077:A:O4'	2.47	0.41
38:n:92:GLY:HA3	51:1:2880:C:H1'	2.03	0.41
47:w:47:VAL:HG21	47:w:76:ILE:HG22	2.02	0.41
51:1:214:G:H1'	51:1:217:A:H5'	2.01	0.41
51:1:910:A:N1	51:1:2277:G:H1'	2.36	0.41
51:1:2472:G:H2'	51:1:2475:C:H42	1.84	0.41
51:1:2739:U:O2'	51:1:2740:A:H5'	2.21	0.41
53:3:1255:G:H2'	53:3:1279:G:H1	1.85	0.41
53:3:1479:C:C4	53:3:1480:A:N7	2.89	0.41
58:B1:576:ARG:HD3	58:B1:593:ASN:HA	2.03	0.41
58:B1:1050:THR:HG23	58:B1:1057:SER:HB3	2.02	0.41
59:B2:27:LEU:O	59:B2:528:ARG:NH1	2.43	0.41
59:B2:1278:LEU:HD23	59:B2:1278:LEU:HA	1.86	0.41
63:6:53:G:H1'	64:a:55:SER:OG	2.21	0.41
65:0:438:LEU:HD11	65:0:472:ARG:HD3	2.03	0.41
11:K:44:ARG:HA	11:K:58:HIS:HA	2.03	0.41
15:O:15:HIS:HD2	53:3:1152:A:H5'	1.86	0.41
16:P:52:ARG:NH1	53:3:689:C:OP2	2.51	0.41
33:i:100:ILE:HB	33:i:139:VAL:HG12	2.02	0.41
33:i:135:MET:SD	51:1:1063:G:H1'	2.60	0.41
42:r:80:ARG:N	51:1:565:C:OP2	2.51	0.41
51:1:399:U:OP1	51:1:2090:A:H5''	2.21	0.41
51:1:610:C:O5'	51:1:610:C:H6	2.03	0.41
51:1:1341:G:H5''	51:1:1397:U:O2	2.21	0.41
51:1:1429:G:H2'	51:1:1430:G:H8	1.85	0.41
51:1:1916:A:H2'	51:1:1917:U:O4'	2.20	0.41
51:1:2528:U:H2'	51:1:2530:A:O5'	2.20	0.41
53:3:215:C:H2'	53:3:216:U:C6	2.56	0.41
53:3:916:U:H2'	53:3:917:G:H8	1.86	0.41
53:3:1448:C:H2'	53:3:1449:C:C6	2.56	0.41
58:B1:109:SER:HA	58:B1:110:PRO:HD3	1.96	0.41
58:B1:390:LEU:HD13	58:B1:390:LEU:H	1.85	0.41
58:B1:820:ILE:HD11	58:B1:822:MET:HE2	2.02	0.41
59:B2:738:GLU:HA	59:B2:741:MET:HE2	2.03	0.41
59:B2:862:LEU:HD22	59:B2:863:SER:N	2.36	0.41
65:0:176:GLU:O	65:0:178:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:1:MET:HB3	1.74	0.41
2:B:7:PRO:HD2	51:1:1263:U:O2'	2.21	0.41
8:H:162:ALA:HB2	53:3:1056:U:C5'	2.48	0.41
9:I:50:TYR:HD2	53:3:509:A:H5''	1.84	0.41
9:I:80:ARG:HG3	53:3:613:C:OP1	2.21	0.41
9:I:145:ARG:HH22	9:I:147:LYS:HD2	1.85	0.41
12:L:83:THR:O	12:L:83:THR:HG22	2.21	0.41
14:N:18:VAL:HG22	14:N:64:ILE:HG23	2.02	0.41
28:c:133:THR:HG21	51:1:1676:A:H1'	2.01	0.41
30:e:65:LEU:HD11	52:2:41:G:H2'	2.02	0.41
31:f:28:LYS:HE2	31:f:28:LYS:HB2	1.92	0.41
31:f:148:ARG:HA	31:f:161:VAL:HB	2.03	0.41
32:g:2:GLN:HE21	32:g:20:ASN:HB2	1.85	0.41
47:w:19:VAL:HG13	47:w:34:VAL:HG22	2.03	0.41
49:y:32:ALA:HB2	49:y:37:LEU:HD23	2.03	0.41
51:1:535:G:H2'	51:1:536:G:O4'	2.20	0.41
51:1:671:C:H2'	51:1:672:C:C6	2.56	0.41
51:1:1508:A:H2'	51:1:1509:A:O4'	2.21	0.41
51:1:1636:U:H2'	51:1:1637:A:C8	2.55	0.41
51:1:1748:C:H2'	51:1:1749:A:H8	1.84	0.41
51:1:1944:U:O2'	51:1:1945:G:H5''	2.21	0.41
51:1:2646:C:O5'	51:1:2646:C:H6	2.03	0.41
51:1:2700:A:H2'	51:1:2701:U:C6	2.56	0.41
53:3:26:A:H61	53:3:558:G:H1'	1.86	0.41
53:3:55:A:C4	65:0:329:PHE:HB3	2.56	0.41
53:3:78:A:H61	53:3:91:U:H3	1.69	0.41
53:3:346:G:H3'	53:3:346:G:N3	2.36	0.41
53:3:546:A:H4'	53:3:548:G:O3'	2.20	0.41
53:3:1230:C:O2'	53:3:1231:G:H5'	2.20	0.41
55:8:14:DC:C2	55:8:15:DC:C5	3.09	0.41
57:A1:44:ARG:HA	57:A1:183:ILE:HD12	2.03	0.41
58:B1:86:GLU:H	58:B1:86:GLU:HG3	1.52	0.41
58:B1:139:LEU:HD23	58:B1:139:LEU:HA	1.89	0.41
58:B1:239:LEU:HD23	58:B1:239:LEU:N	2.36	0.41
59:B2:657:THR:HG21	59:B2:1188:ASP:HB2	2.03	0.41
59:B2:678:ARG:HA	59:B2:678:ARG:HD3	1.84	0.41
59:B2:870:ILE:HB	59:B2:944:ARG:HD3	2.02	0.41
65:0:145:ASP:CG	68:0:801:GDP:HN21	2.29	0.41
65:0:200:VAL:HG23	65:0:201:THR:HG23	2.02	0.41
65:0:521:ASP:HB2	65:0:579:HIS:HD2	1.86	0.41
1:A:27:THR:OG1	30:e:58:ALA:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:46:LYS:H	20:T:46:LYS:HG3	1.64	0.41
27:b:129:LEU:HD12	27:b:133:ASN:HB2	2.03	0.41
27:b:179:GLU:HB2	27:b:270:ARG:HB3	2.02	0.41
28:c:47:ALA:HA	28:c:84:LEU:HG	2.04	0.41
42:r:85:LYS:HE3	51:1:815:C:OP2	2.20	0.41
44:t:8:LEU:O	49:y:29:ARG:NH1	2.53	0.41
49:y:19:LEU:HA	49:y:23:ARG:HH21	1.86	0.41
51:1:732:C:H2'	51:1:733:G:O4'	2.21	0.41
51:1:1091:G:H2'	51:1:1092:C:C6	2.56	0.41
51:1:2360:G:H2'	51:1:2361:G:O4'	2.21	0.41
53:3:20:U:H2'	53:3:21:G:O4'	2.20	0.41
57:A1:224:LEU:HD23	57:A2:228:LEU:HD21	2.03	0.41
57:A2:57:THR:HG23	57:A2:158:ARG:HH21	1.86	0.41
58:B1:68:TYR:CB	58:B1:75:TYR:HE2	2.34	0.41
58:B1:395:LYS:HB3	58:B1:395:LYS:HE3	1.45	0.41
59:B2:864:LYS:HD3	59:B2:877:VAL:HG12	2.03	0.41
59:B2:979:LEU:HD11	59:B2:1011:LEU:HD11	2.03	0.41
62:5:17:C:H2'	62:5:18:G:C8	2.56	0.41
65:0:197:ASP:C	65:0:199:GLY:H	2.29	0.41
21:U:4:ILE:HD12	21:U:67:ILE:HG13	2.03	0.40
21:U:79:ASN:OD1	21:U:79:ASN:N	2.53	0.40
27:b:144:GLU:OE1	27:b:150:GLY:N	2.54	0.40
27:b:211:ARG:HD3	27:b:217:PRO:HD3	2.03	0.40
28:c:29:VAL:HB	28:c:98:VAL:HG22	2.02	0.40
29:d:131:THR:HG23	51:1:321:U:H5''	2.03	0.40
36:l:63:LYS:HE3	51:1:2394:C:H5''	2.03	0.40
41:q:24:TYR:HE1	51:1:17:G:H4'	1.85	0.40
43:s:97:LEU:HD23	43:s:97:LEU:HA	1.90	0.40
44:t:1:MET:HE2	51:1:136:G:H21	1.85	0.40
51:1:272:A:H2'	51:1:273:G:H8	1.86	0.40
51:1:859:G:O2'	51:1:860:U:H6	2.04	0.40
51:1:1137:G:H2'	51:1:1138:G:H8	1.85	0.40
51:1:1757:A:O5'	51:1:1757:A:H8	2.04	0.40
51:1:2548:U:C4	51:1:2549:G:N7	2.88	0.40
51:1:2853:C:H2'	51:1:2854:G:H8	1.86	0.40
53:3:26:A:N6	53:3:558:G:H1'	2.36	0.40
53:3:78:A:H8	53:3:78:A:O5'	2.05	0.40
53:3:812:G:OP1	53:3:903:G:H1'	2.21	0.40
53:3:1201:A:H4'	53:3:1202:U:C5'	2.49	0.40
55:8:2:DC:C6	55:8:2:DC:H5'	2.56	0.40
57:A2:104:LYS:HG2	57:A2:110:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:394:ILE:O	58:B1:394:ILE:HG13	2.19	0.40
59:B2:11:ILE:O	59:B2:1149:TYR:OH	2.27	0.40
59:B2:886:LYS:HE2	59:B2:918:LEU:HD13	2.03	0.40
65:0:352:SER:OG	65:0:396:THR:O	2.33	0.40
1:A:64:PHE:HA	53:3:1011:C:H5'	2.03	0.40
12:L:3:ARG:HB3	12:L:4:ARG:HH11	1.87	0.40
22:V:13:SER:O	22:V:13:SER:OG	2.34	0.40
28:c:16:THR:OG1	28:c:18:ASP:OD1	2.35	0.40
31:f:159:LYS:NZ	51:1:2657:A:O2'	2.53	0.40
34:j:132:HIS:ND1	51:1:7:G:H5'	2.36	0.40
35:k:44:LYS:HA	35:k:44:LYS:HD3	1.95	0.40
35:k:95:ILE:H	35:k:95:ILE:HG13	1.62	0.40
51:1:4:U:H2'	51:1:5:A:C8	2.56	0.40
51:1:94:A:H2'	51:1:95:A:O4'	2.21	0.40
51:1:123:G:H4'	51:1:1376:C:O5'	2.21	0.40
51:1:284:U:H2'	51:1:285:G:C8	2.55	0.40
51:1:631:A:H1'	51:1:2415:G:O2'	2.21	0.40
51:1:1808:A:H3'	51:1:1809:A:C8	2.56	0.40
53:3:471:U:H2'	53:3:472:U:C6	2.56	0.40
53:3:619:U:H3'	53:3:619:U:H6	1.86	0.40
53:3:623:C:H2'	53:3:624:C:C6	2.56	0.40
58:B1:245:LEU:HD13	59:B2:1329:GLU:HA	2.04	0.40
58:B1:1106:ILE:O	58:B1:1123:ARG:N	2.45	0.40
59:B2:310:ILE:HG21	59:B2:325:LEU:HB3	2.03	0.40
64:a:200:LYS:HB2	64:a:200:LYS:HE2	1.87	0.40
65:0:230:SER:HB2	65:0:233:LEU:HB3	2.03	0.40
1:A:1:MET:HB2	52:2:43:C:OP1	2.20	0.40
12:L:24:LYS:HD2	12:L:24:LYS:HA	1.96	0.40
12:L:65:LEU:HA	12:L:68:VAL:HG12	2.03	0.40
25:Y:66:ILE:HG23	25:Y:70:LYS:HD3	2.01	0.40
26:Z:7:GLU:HG3	26:Z:15:LEU:HB2	2.02	0.40
27:b:211:ARG:HG3	51:1:764:A:N3	2.36	0.40
34:j:109:LEU:HD23	34:j:109:LEU:HA	1.87	0.40
35:k:9:ASN:HD22	35:k:9:ASN:HA	1.70	0.40
46:v:26:PHE:HE2	46:v:89:ILE:HG13	1.87	0.40
51:1:179:C:O2'	51:1:180:G:H5'	2.21	0.40
51:1:227:A:H1'	51:1:229:C:H41	1.86	0.40
51:1:558:U:H2'	51:1:559:G:C8	2.54	0.40
51:1:1380:G:O5'	51:1:1380:G:C8	2.74	0.40
51:1:1507:C:H2'	51:1:1508:A:O4'	2.21	0.40
51:1:1747:U:H2'	51:1:1748:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2004:G:H2'	51:1:2005:A:O4'	2.21	0.40
51:1:2011:U:H2'	51:1:2012:G:O4'	2.22	0.40
53:3:401:C:H2'	53:3:402:G:C8	2.56	0.40
53:3:702:A:H2'	53:3:702:A:N3	2.37	0.40
53:3:876:C:H2'	53:3:877:G:H8	1.86	0.40
57:A2:42:ALA:HB1	57:A2:224:LEU:HD11	2.03	0.40
58:B1:71:LEU:HB2	58:B1:90:VAL:HG11	2.03	0.40
59:B2:213:LEU:HD13	59:B2:422:LYS:HG2	2.03	0.40
59:B2:741:MET:SD	59:B2:974:ARG:NH2	2.93	0.40
1:A:63:ARG:NH1	53:3:1013:G:OP2	2.54	0.40
4:D:19:ARG:NH2	51:1:124:G:C5	2.89	0.40
8:H:128:MET:HE2	8:H:128:MET:HB2	1.65	0.40
16:P:52:ARG:HH22	53:3:689:C:H5	1.68	0.40
20:T:11:VAL:HG23	20:T:26:VAL:HG11	2.04	0.40
23:W:47:ARG:H	23:W:47:ARG:HG2	1.60	0.40
27:b:68:ARG:O	27:b:188:ARG:NH2	2.55	0.40
32:g:8:LYS:HG3	32:g:14:SER:HA	2.04	0.40
36:l:62:PRO:HG3	51:1:2393:U:H5''	2.04	0.40
42:r:16:GLU:HG2	42:r:101:ILE:HG12	2.04	0.40
51:1:839:U:H2'	51:1:840:C:C6	2.56	0.40
51:1:935:C:H2'	51:1:936:A:H8	1.87	0.40
51:1:987:C:H2'	51:1:988:A:O4'	2.21	0.40
51:1:1139:G:H8	51:1:1139:G:O5'	2.04	0.40
51:1:1461:C:O5'	51:1:1461:C:H6	2.05	0.40
51:1:2441:U:H2'	51:1:2442:C:H6	1.87	0.40
53:3:37:U:H2'	53:3:38:G:O4'	2.21	0.40
55:8:22:DC:H2'	58:B1:259:ARG:HH22	1.87	0.40
57:A1:79:LEU:HD11	58:B1:526:VAL:HG21	2.04	0.40
58:B1:117:LEU:HD22	58:B1:139:LEU:CD1	2.52	0.40
64:a:167:LYS:HE2	64:a:167:LYS:HB2	1.76	0.40
66:h:5:UAL:C	66:h:6:5OH:HS	2.52	0.40
7:G:203:ASP:OD1	7:G:203:ASP:N	2.54	0.40
10:J:24:VAL:HG12	10:J:25:LYS:H	1.87	0.40
14:N:71:ILE:O	14:N:75:ALA:N	2.52	0.40
16:P:33:ILE:HG22	16:P:41:LEU:HD12	2.04	0.40
18:R:95:PRO:HD3	18:R:108:ARG:HB3	2.04	0.40
46:v:80:HIS:H	46:v:86:LEU:HA	1.86	0.40
51:1:1866:A:H2'	51:1:1867:G:O4'	2.20	0.40
51:1:2722:G:H8	51:1:2722:G:O5'	2.05	0.40
53:3:179:A:H61	53:3:196:A:H62	1.69	0.40
53:3:216:U:O3'	53:3:464:U:H4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:404:G:H2'	53:3:405:U:C6	2.55	0.40
53:3:865:A:H5'	53:3:1078:U:C4	2.57	0.40
58:B1:351:GLY:O	58:B1:467:ALA:HA	2.22	0.40
58:B1:472:LEU:HD11	59:B2:1294:LYS:HG2	2.03	0.40
58:B1:907:HIS:ND1	58:B1:908:ILE:O	2.53	0.40
59:B2:805:MET:HB2	59:B2:805:MET:HE3	1.86	0.40
62:5:37:A:H3'	62:5:38:A:C8	2.56	0.40
65:0:68:THR:HG22	65:0:69:THR:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
2	B	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
3	C	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
4	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
5	E	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
6	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	187 (87%)	29 (13%)	0	100	100
8	H	204/233 (88%)	181 (89%)	22 (11%)	1 (0%)	25	64
9	I	203/206 (98%)	178 (88%)	25 (12%)	0	100	100
10	J	155/167 (93%)	133 (86%)	21 (14%)	1 (1%)	22	60
11	K	98/135 (73%)	83 (85%)	14 (14%)	1 (1%)	13	49
12	L	149/179 (83%)	130 (87%)	17 (11%)	2 (1%)	10	43
13	M	127/130 (98%)	120 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	125/130 (96%)	97 (78%)	26 (21%)	2 (2%)	8	38
15	O	96/103 (93%)	77 (80%)	18 (19%)	1 (1%)	13	49
16	P	114/129 (88%)	90 (79%)	22 (19%)	2 (2%)	7	35
17	Q	121/124 (98%)	100 (83%)	18 (15%)	3 (2%)	4	26
18	R	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	52
19	S	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	22
20	T	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
21	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	43
22	V	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	10	43
23	W	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
24	X	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
25	Y	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
26	Z	63/71 (89%)	45 (71%)	18 (29%)	0	100	100
27	b	269/273 (98%)	233 (87%)	31 (12%)	5 (2%)	6	32
28	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	25	64
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
31	f	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	7	37
32	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	19	57
33	i	139/142 (98%)	115 (83%)	23 (16%)	1 (1%)	19	57
34	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	19	57
35	k	120/123 (98%)	100 (83%)	20 (17%)	0	100	100
36	l	141/144 (98%)	121 (86%)	20 (14%)	0	100	100
37	m	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
38	n	118/127 (93%)	101 (86%)	17 (14%)	0	100	100
39	o	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	14	52
40	p	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
42	r	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
43	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
44	t	91/100 (91%)	78 (86%)	13 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	u	100/104 (96%)	81 (81%)	18 (18%)	1 (1%)	13	49
46	v	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
47	w	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
48	x	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
49	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	38
50	z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
57	A1	214/329 (65%)	195 (91%)	19 (9%)	0	100	100
57	A2	217/329 (66%)	206 (95%)	11 (5%)	0	100	100
58	B1	1329/1407 (94%)	1206 (91%)	119 (9%)	4 (0%)	37	73
59	B2	1338/1342 (100%)	1204 (90%)	129 (10%)	5 (0%)	30	68
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NG	84/181 (46%)	77 (92%)	6 (7%)	1 (1%)	11	45
64	a	130/234 (56%)	112 (86%)	18 (14%)	0	100	100
65	0	695/716 (97%)	621 (89%)	71 (10%)	3 (0%)	30	68
66	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	9806/10690 (92%)	8733 (89%)	1026 (10%)	47 (0%)	27	64

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q	87	LYS
31	f	45	ALA
32	g	136	SER
49	y	24	GLU
58	B1	121	PRO
11	K	56	LYS
17	Q	102	ASP
19	S	60	ARG
21	U	45	GLU
27	b	46	GLY
28	c	197	THR
33	i	121	ILE
59	B2	43	PRO
59	B2	918	LEU
61	NG	102	PRO
65	0	176	GLU
65	0	177	GLU

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Mol	Chain	Res	Type
12	L	6	ILE
17	Q	101	LEU
19	S	61	ASN
27	b	205	GLY
39	o	34	HIS
59	B2	888	THR
14	N	23	GLY
16	P	89	GLY
22	V	50	ASN
31	f	44	HIS
58	B1	43	THR
58	B1	193	ASP
14	N	102	PHE
27	b	255	LYS
31	f	174	LYS
45	u	6	ARG
58	B1	1325	PHE
65	0	198	GLN
16	P	88	PRO
18	R	7	ASN
19	S	35	ALA
59	B2	857	VAL
34	j	110	PRO
12	L	79	VAL
27	b	232	GLY
8	H	12	GLY
27	b	240	GLY
59	B2	1317	PRO
10	J	97	PRO
15	O	57	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/62 (95%)	56 (95%)	3 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	47/48 (98%)	45 (96%)	2 (4%)	25	46
3	C	45/49 (92%)	45 (100%)	0	100	100
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	59
5	E	51/52 (98%)	48 (94%)	3 (6%)	16	37
6	F	34/34 (100%)	34 (100%)	0	100	100
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	52
8	H	169/190 (89%)	158 (94%)	11 (6%)	14	35
9	I	172/173 (99%)	165 (96%)	7 (4%)	26	47
10	J	118/126 (94%)	114 (97%)	4 (3%)	32	51
11	K	87/116 (75%)	83 (95%)	4 (5%)	23	44
12	L	124/147 (84%)	122 (98%)	2 (2%)	58	74
13	M	104/105 (99%)	104 (100%)	0	100	100
14	N	105/107 (98%)	95 (90%)	10 (10%)	7	22
15	O	86/90 (96%)	77 (90%)	9 (10%)	5	19
16	P	89/99 (90%)	88 (99%)	1 (1%)	70	80
17	Q	103/104 (99%)	93 (90%)	10 (10%)	6	22
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	82 (99%)	1 (1%)	67	79
20	T	76/77 (99%)	71 (93%)	5 (7%)	14	34
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	73 (99%)	1 (1%)	62	75
23	W	56/65 (86%)	54 (96%)	2 (4%)	30	50
24	X	70/79 (89%)	69 (99%)	1 (1%)	62	75
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	52 (94%)	3 (6%)	18	39
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	162 (99%)	2 (1%)	67	79
29	d	165/165 (100%)	163 (99%)	2 (1%)	67	79
30	e	148/150 (99%)	144 (97%)	4 (3%)	40	58
31	f	137/138 (99%)	137 (100%)	0	100	100
32	g	114/114 (100%)	112 (98%)	2 (2%)	54	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	i	109/110 (99%)	95 (87%)	14 (13%)	3	14
34	j	116/116 (100%)	115 (99%)	1 (1%)	75	83
35	k	103/104 (99%)	96 (93%)	7 (7%)	13	34
36	l	102/103 (99%)	100 (98%)	2 (2%)	50	68
37	m	109/109 (100%)	109 (100%)	0	100	100
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	82
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	97 (98%)	2 (2%)	50	68
41	q	89/90 (99%)	84 (94%)	5 (6%)	17	38
42	r	84/84 (100%)	81 (96%)	3 (4%)	30	50
43	s	93/93 (100%)	93 (100%)	0	100	100
44	t	80/84 (95%)	79 (99%)	1 (1%)	65	77
45	u	82/85 (96%)	81 (99%)	1 (1%)	67	79
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	56 (98%)	1 (2%)	54	71
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	25	46
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	37
57	A2	186/286 (65%)	186 (100%)	0	100	100
58	B1	1110/1168 (95%)	1020 (92%)	90 (8%)	9	28
59	B2	1137/1157 (98%)	1111 (98%)	26 (2%)	45	64
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
64	a	110/181 (61%)	110 (100%)	0	100	100
65	0	574/588 (98%)	546 (95%)	28 (5%)	21	42
66	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8122/8683 (94%)	7823 (96%)	299 (4%)	31	49

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	ASP

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Mol	Chain	Res	Type
1	A	57	VAL
2	B	2	VAL
2	B	21	LEU
4	D	43	THR
5	E	30	HIS
5	E	32	LEU
5	E	34	LYS
7	G	17	HIS
7	G	19	THR
7	G	20	ARG
7	G	46	VAL
7	G	48	MET
7	G	160	LEU
8	H	62	SER
8	H	63	ILE
8	H	78	LYS
8	H	79	LYS
8	H	81	GLU
8	H	104	GLU
8	H	124	GLU
8	H	126	ARG
8	H	128	MET
8	H	156	LEU
8	H	172	VAL
9	I	27	ILE
9	I	28	ASP
9	I	29	THR
9	I	30	LYS
9	I	32	LYS
9	I	33	ILE
9	I	170	LEU
10	J	75	LEU
10	J	120	HIS
10	J	121	ASN
10	J	123	LEU
11	K	47	LEU
11	K	53	LYS
11	K	92	THR
11	K	93	LYS
12	L	29	LEU
12	L	134	VAL
14	N	20	ILE

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Mol	Chain	Res	Type
14	N	21	LYS
14	N	24	ASN
14	N	54	VAL
14	N	55	ASP
14	N	56	MET
14	N	57	VAL
14	N	59	LYS
14	N	89	TYR
14	N	91	GLU
15	O	78	GLU
15	O	82	LYS
15	O	84	VAL
15	O	88	MET
15	O	89	ARG
15	O	90	LEU
15	O	92	LEU
15	O	99	GLN
15	O	102	LEU
16	P	15	VAL
17	Q	2	THR
17	Q	3	VAL
17	Q	20	VAL
17	Q	24	GLU
17	Q	26	CYS
17	Q	42	LYS
17	Q	43	LYS
17	Q	45	ASN
17	Q	97	VAL
17	Q	107	LYS
18	R	82	LEU
19	S	78	LEU
20	T	44	GLU
20	T	46	LYS
20	T	47	LYS
20	T	48	ASP
20	T	55	LEU
21	U	19	VAL
22	V	40	THR
23	W	28	LEU
23	W	47	ARG
24	X	38	THR
26	Z	24	LYS

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Mol	Chain	Res	Type
26	Z	35	GLU
26	Z	40	PRO
27	b	12	ARG
27	b	18	VAL
27	b	171	VAL
27	b	194	VAL
28	c	79	LEU
28	c	98	VAL
29	d	79	ARG
29	d	80	SER
30	e	108	PRO
30	e	174	PHE
30	e	176	PHE
30	e	177	ARG
32	g	5	LEU
32	g	143	ILE
33	i	2	LYS
33	i	3	LYS
33	i	5	GLN
33	i	18	ASN
33	i	23	VAL
33	i	27	LEU
33	i	29	GLN
33	i	67	THR
33	i	72	THR
33	i	117	THR
33	i	124	MET
33	i	131	THR
33	i	134	SER
33	i	135	MET
34	j	10	THR
35	k	61	VAL
35	k	85	VAL
35	k	86	LEU
35	k	90	ASN
35	k	92	GLU
35	k	93	GLN
35	k	95	ILE
36	l	85	VAL
36	l	127	VAL
38	n	50	PRO
40	p	32	VAL

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Mol	Chain	Res	Type
40	p	109	ILE
41	q	5	ARG
41	q	7	VAL
41	q	82	LEU
41	q	84	LYS
41	q	86	SER
42	r	48	LYS
42	r	49	ILE
42	r	55	ASP
44	t	67	VAL
45	u	27	VAL
46	v	70	ILE
47	w	19	VAL
50	z	10	ARG
50	z	15	ARG
57	A1	9	LEU
57	A1	12	ARG
57	A1	13	LEU
57	A1	18	GLN
57	A1	19	VAL
57	A1	22	THR
57	A1	27	THR
57	A1	28	LEU
57	A1	33	ARG
57	A1	46	ILE
57	A1	48	LEU
58	B1	24	LEU
58	B1	40	LYS
58	B1	42	GLU
58	B1	44	ILE
58	B1	47	ARG
58	B1	49	PHE
58	B1	50	LYS
58	B1	60	ARG
58	B1	66	LYS
58	B1	69	GLU
58	B1	71	LEU
58	B1	74	LYS
58	B1	76	LYS
58	B1	78	LEU
58	B1	80	HIS
58	B1	81	ARG

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Mol	Chain	Res	Type
58	B1	86	GLU
58	B1	87	LYS
58	B1	91	GLU
58	B1	93	THR
58	B1	94	GLN
58	B1	95	THR
58	B1	96	LYS
58	B1	99	ARG
58	B1	100	GLU
58	B1	114	ILE
58	B1	117	LEU
58	B1	120	LEU
58	B1	126	LEU
58	B1	132	LEU
58	B1	135	ILE
58	B1	142	GLU
58	B1	144	TYR
58	B1	145	VAL
58	B1	146	VAL
58	B1	147	ILE
58	B1	152	THR
58	B1	154	LEU
58	B1	157	GLN
58	B1	159	ILE
58	B1	172	PHE
58	B1	174	ASP
58	B1	175	GLU
58	B1	180	MET
58	B1	190	LYS
58	B1	193	ASP
58	B1	196	GLN
58	B1	210	SER
58	B1	212	THR
58	B1	216	LYS
58	B1	222	LYS
58	B1	223	LEU
58	B1	227	PHE
58	B1	233	LYS
58	B1	237	MET
58	B1	238	ILE
58	B1	239	LEU
58	B1	240	THR

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Mol	Chain	Res	Type
58	B1	244	VAL
58	B1	255	LEU
58	B1	256	ASP
58	B1	259	ARG
58	B1	317	THR
58	B1	322	ARG
58	B1	324	LEU
58	B1	363	LEU
58	B1	385	LEU
58	B1	386	GLU
58	B1	387	LEU
58	B1	390	LEU
58	B1	393	THR
58	B1	394	ILE
58	B1	395	LYS
58	B1	416	ILE
58	B1	417	ARG
58	B1	425	ARG
58	B1	506	VAL
58	B1	514	THR
58	B1	800	LEU
58	B1	807	LEU
58	B1	839	VAL
58	B1	901	ARG
58	B1	903	LEU
58	B1	1172	LYS
58	B1	1181	ASP
58	B1	1233	ILE
58	B1	1327	GLU
58	B1	1328	THR
58	B1	1331	VAL
58	B1	1332	LEU
59	B2	44	GLU
59	B2	49	LEU
59	B2	56	VAL
59	B2	146	VAL
59	B2	483	ASP
59	B2	487	LEU
59	B2	516	ASP
59	B2	538	LEU
59	B2	540	ARG
59	B2	545	PHE

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Mol	Chain	Res	Type
59	B2	546	GLU
59	B2	615	VAL
59	B2	857	VAL
59	B2	862	LEU
59	B2	864	LYS
59	B2	867	GLU
59	B2	872	TYR
59	B2	876	GLU
59	B2	887	VAL
59	B2	890	LYS
59	B2	912	ASP
59	B2	918	LEU
59	B2	920	VAL
59	B2	922	ASN
59	B2	1076	ILE
59	B2	1151	LEU
60	W0	63	ILE
65	0	31	LEU
65	0	97	ILE
65	0	214	LEU
65	0	360	PHE
65	0	415	VAL
65	0	418	ILE
65	0	483	VAL
65	0	485	LYS
65	0	488	VAL
65	0	507	LYS
65	0	512	ARG
65	0	519	VAL
65	0	522	MET
65	0	525	LEU
65	0	526	GLU
65	0	551	PRO
65	0	584	HIS
65	0	626	GLU
65	0	627	ASN
65	0	628	THR
65	0	630	ASP
65	0	636	SER
65	0	638	ARG
65	0	642	LEU
65	0	643	LYS

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Mol	Chain	Res	Type
65	0	646	GLU
65	0	648	GLU
65	0	649	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
2	B	3	GLN
2	B	5	ASN
4	D	26	ASN
5	E	30	HIS
7	G	17	HIS
7	G	57	ASN
7	G	93	HIS
7	G	176	ASN
8	H	138	GLN
8	H	139	ASN
9	I	53	GLN
9	I	58	GLN
9	I	84	ASN
10	J	88	HIS
10	J	131	ASN
10	J	145	ASN
10	J	147	ASN
12	L	121	ASN
12	L	147	ASN
13	M	66	GLN
14	N	4	GLN
14	N	24	ASN
14	N	30	ASN
14	N	31	GLN
15	O	15	HIS
15	O	35	GLN
16	P	27	ASN
16	P	37	GLN
16	P	39	ASN
16	P	63	GLN
16	P	100	ASN
17	Q	5	GLN
17	Q	45	ASN
17	Q	76	HIS

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Mol	Chain	Res	Type
17	Q	95	HIS
18	R	13	HIS
19	S	48	GLN
20	T	27	GLN
20	T	49	HIS
21	U	26	ASN
21	U	63	GLN
23	W	51	GLN
25	Y	54	GLN
25	Y	67	HIS
25	Y	69	ASN
25	Y	74	HIS
26	Z	63	ASN
27	b	24	HIS
27	b	45	ASN
27	b	57	HIS
27	b	114	GLN
27	b	152	GLN
28	c	42	ASN
28	c	49	GLN
28	c	58	ASN
28	c	136	ASN
28	c	164	GLN
29	d	94	GLN
29	d	97	ASN
29	d	163	ASN
30	e	26	GLN
31	f	63	GLN
31	f	87	GLN
31	f	103	ASN
31	f	110	HIS
31	f	142	GLN
32	g	11	ASN
32	g	73	ASN
33	i	110	GLN
34	j	40	HIS
34	j	135	GLN
35	k	3	GLN
35	k	9	ASN
36	l	99	ASN
37	m	3	GLN
37	m	17	ASN

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Mol	Chain	Res	Type
37	m	97	GLN
38	n	9	GLN
38	n	73	ASN
38	n	81	ASN
39	o	61	GLN
39	o	98	GLN
40	p	55	HIS
40	p	74	GLN
41	q	43	GLN
41	q	70	GLN
42	r	11	GLN
42	r	89	HIS
43	s	57	ASN
44	t	15	HIS
44	t	48	GLN
44	t	59	ASN
45	u	68	ASN
46	v	49	ASN
46	v	78	GLN
47	w	8	ASN
47	w	53	HIS
48	x	22	ASN
48	x	35	HIS
49	y	20	ASN
49	y	25	GLN
49	y	31	GLN
50	z	8	GLN
57	A1	37	HIS
57	A1	66	HIS
57	A1	84	ASN
57	A1	117	HIS
57	A1	128	HIS
57	A1	227	GLN
57	A2	23	HIS
57	A2	227	GLN
58	B1	45	ASN
58	B1	364	HIS
58	B1	424	ASN
58	B1	469	HIS
58	B1	805	GLN
58	B1	817	HIS
58	B1	865	HIS

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Mol	Chain	Res	Type
58	B1	1195	GLN
58	B1	1238	GLN
58	B1	1259	GLN
59	B2	69	GLN
59	B2	314	ASN
59	B2	330	HIS
59	B2	343	HIS
59	B2	518	ASN
59	B2	554	HIS
59	B2	688	GLN
59	B2	762	ASN
59	B2	808	ASN
59	B2	1080	ASN
59	B2	1237	HIS
59	B2	1268	GLN
59	B2	1313	HIS
60	W0	7	GLN
60	W0	31	GLN
60	W0	62	GLN
64	a	24	ASN
64	a	47	ASN
64	a	203	GLN
65	0	44	HIS
65	0	85	ASN
65	0	157	GLN
65	0	272	ASN
65	0	296	ASN
65	0	344	ASN
65	0	365	GLN
65	0	428	GLN
65	0	505	HIS
65	0	517	HIS
65	0	530	ASN
65	0	579	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	419 (14%)	10 (0%)
52	2	119/120 (99%)	12 (10%)	1 (0%)
53	3	1538/1542 (99%)	182 (11%)	6 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	4	16/27 (59%)	2 (12%)	0
62	5	75/76 (98%)	38 (50%)	7 (9%)
63	6	76/77 (98%)	18 (23%)	0
All	All	4726/4746 (99%)	671 (14%)	24 (0%)

All (671) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	35	G
51	1	42	A
51	1	46	G
51	1	51	G
51	1	63	A
51	1	71	A
51	1	74	A
51	1	75	G
51	1	98	G
51	1	102	U
51	1	103	A
51	1	119	A
51	1	120	U
51	1	139	U
51	1	140	C
51	1	141	G
51	1	142	A
51	1	149	A
51	1	162	U
51	1	163	C
51	1	181	A
51	1	196	A
51	1	215	G
51	1	216	A
51	1	219	A
51	1	221	A
51	1	222	A
51	1	228	C
51	1	229	C
51	1	232	G
51	1	233	A
51	1	248	G

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Mol	Chain	Res	Type
51	1	255	A
51	1	266	G
51	1	276	U
51	1	278	A
51	1	281	C
51	1	285	G
51	1	294	A
51	1	311	A
51	1	323	C
51	1	324	A
51	1	329	G
51	1	330	A
51	1	346	A
51	1	353	C
51	1	361	G
51	1	362	A
51	1	371	A
51	1	372	G
51	1	386	G
51	1	387	U
51	1	404	A
51	1	405	U
51	1	411	G
51	1	412	A
51	1	424	G
51	1	451	U
51	1	455	C
51	1	456	C
51	1	481	G
51	1	491	G
51	1	504	A
51	1	508	A
51	1	528	A
51	1	531	C
51	1	532	A
51	1	533	G
51	1	544	C
51	1	545	U
51	1	563	A
51	1	572	A
51	1	573	U
51	1	586	A

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Mol	Chain	Res	Type
51	1	588	U
51	1	603	A
51	1	614	A
51	1	627	A
51	1	637	A
51	1	646	U
51	1	654	A
51	1	655	A
51	1	664	G
51	1	686	U
51	1	687	C
51	1	695	G
51	1	717	C
51	1	730	A
51	1	740	C
51	1	747	C
51	1	748	G
51	1	749	A
51	1	760	G
51	1	764	A
51	1	774	G
51	1	776	G
51	1	782	A
51	1	784	G
51	1	785	G
51	1	803	U
51	1	805	G
51	1	812	C
51	1	819	A
51	1	827	U
51	1	828	U
51	1	830	G
51	1	845	A
51	1	846	U
51	1	856	G
51	1	858	G
51	1	860	U
51	1	869	G
51	1	871	U
51	1	872	U
51	1	877	A
51	1	878	A

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Mol	Chain	Res	Type
51	1	885	C
51	1	887	U
51	1	896	A
51	1	897	C
51	1	907	G
51	1	910	A
51	1	914	G
51	1	915	C
51	1	932	U
51	1	934	U
51	1	941	A
51	1	946	C
51	1	961	C
51	1	974	G
51	1	975	A
51	1	983	A
51	1	985	C
51	1	995	C
51	1	1012	U
51	1	1013	C
51	1	1021	A
51	1	1022	G
51	1	1023	U
51	1	1026	G
51	1	1033	U
51	1	1034	G
51	1	1045	C
51	1	1046	A
51	1	1047	G
51	1	1053	C
51	1	1055	G
51	1	1057	A
51	1	1058	U
51	1	1059	G
51	1	1062	G
51	1	1064	C
51	1	1065	U
51	1	1066	U
51	1	1069	A
51	1	1070	A
51	1	1071	G
51	1	1072	C

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Mol	Chain	Res	Type
51	1	1073	A
51	1	1076	C
51	1	1078	U
51	1	1080	A
51	1	1081	U
51	1	1082	U
51	1	1083	U
51	1	1084	A
51	1	1085	A
51	1	1086	A
51	1	1087	G
51	1	1088	A
51	1	1092	C
51	1	1104	C
51	1	1105	U
51	1	1106	G
51	1	1111	A
51	1	1131	G
51	1	1132	U
51	1	1133	A
51	1	1135	C
51	1	1143	A
51	1	1157	G
51	1	1172	C
51	1	1173	U
51	1	1175	A
51	1	1177	G
51	1	1179	G
51	1	1180	U
51	1	1211	C
51	1	1212	G
51	1	1221	C
51	1	1248	G
51	1	1249	U
51	1	1253	A
51	1	1256	G
51	1	1271	G
51	1	1272	A
51	1	1273	U
51	1	1275	A
51	1	1289	C
51	1	1300	G

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Mol	Chain	Res	Type
51	1	1301	A
51	1	1341	G
51	1	1345	C
51	1	1352	U
51	1	1365	A
51	1	1378	A
51	1	1379	U
51	1	1383	A
51	1	1398	C
51	1	1416	G
51	1	1419	A
51	1	1420	A
51	1	1427	A
51	1	1428	C
51	1	1458	U
51	1	1478	G
51	1	1482	G
51	1	1490	A
51	1	1491	G
51	1	1493	C
51	1	1504	A
51	1	1515	A
51	1	1524	G
51	1	1533	C
51	1	1534	U
51	1	1535	A
51	1	1536	C
51	1	1537	G
51	1	1555	G
51	1	1558	C
51	1	1559	U
51	1	1560	G
51	1	1569	A
51	1	1578	U
51	1	1584	U
51	1	1608	A
51	1	1611	C
51	1	1616	A
51	1	1618	A
51	1	1647	U
51	1	1648	U
51	1	1654	A

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Mol	Chain	Res	Type
51	1	1674	G
51	1	1682	G
51	1	1698	A
51	1	1715	G
51	1	1729	U
51	1	1730	C
51	1	1732	C
51	1	1733	G
51	1	1738	G
51	1	1758	U
51	1	1764	C
51	1	1773	A
51	1	1780	A
51	1	1785	A
51	1	1791	A
51	1	1800	C
51	1	1801	A
51	1	1808	A
51	1	1816	C
51	1	1820	U
51	1	1821	A
51	1	1829	A
51	1	1839	G
51	1	1857	G
51	1	1869	G
51	1	1870	C
51	1	1871	A
51	1	1901	A
51	1	1906	G
51	1	1907	G
51	1	1912	A
51	1	1913	A
51	1	1914	C
51	1	1925	C
51	1	1929	G
51	1	1930	G
51	1	1937	A
51	1	1938	A
51	1	1944	U
51	1	1955	U
51	1	1961	C
51	1	1963	U

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Mol	Chain	Res	Type
51	1	1967	C
51	1	1970	A
51	1	1971	U
51	1	1972	G
51	1	1991	U
51	1	1992	G
51	1	1993	U
51	1	1996	C
51	1	1997	C
51	1	2022	U
51	1	2023	C
51	1	2030	A
51	1	2031	A
51	1	2043	C
51	1	2055	C
51	1	2056	G
51	1	2060	A
51	1	2061	G
51	1	2062	A
51	1	2069	G
51	1	2072	C
51	1	2077	A
51	1	2092	U
51	1	2095	A
51	1	2096	C
51	1	2100	G
51	1	2106	U
51	1	2111	U
51	1	2112	G
51	1	2118	U
51	1	2119	A
51	1	2120	G
51	1	2122	U
51	1	2125	G
51	1	2128	G
51	1	2132	U
51	1	2133	G
51	1	2134	A
51	1	2138	G
51	1	2141	G
51	1	2145	C
51	1	2153	C

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Mol	Chain	Res	Type
51	1	2158	A
51	1	2162	G
51	1	2166	U
51	1	2172	U
51	1	2173	A
51	1	2178	C
51	1	2182	U
51	1	2184	A
51	1	2192	U
51	1	2198	A
51	1	2203	U
51	1	2204	G
51	1	2211	A
51	1	2225	A
51	1	2239	G
51	1	2278	A
51	1	2283	C
51	1	2287	A
51	1	2297	A
51	1	2305	U
51	1	2309	A
51	1	2325	G
51	1	2327	A
51	1	2333	A
51	1	2337	G
51	1	2350	C
51	1	2385	C
51	1	2402	U
51	1	2406	A
51	1	2423	U
51	1	2425	A
51	1	2426	A
51	1	2427	C
51	1	2428	G
51	1	2429	G
51	1	2430	A
51	1	2435	A
51	1	2441	U
51	1	2447	G
51	1	2448	A
51	1	2469	A
51	1	2474	U

*Continued on next page...*

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Mol	Chain	Res	Type
51	1	2476	A
51	1	2480	C
51	1	2491	U
51	1	2502	G
51	1	2505	G
51	1	2518	A
51	1	2529	G
51	1	2535	G
51	1	2547	A
51	1	2554	U
51	1	2566	A
51	1	2567	G
51	1	2572	A
51	1	2602	A
51	1	2603	G
51	1	2609	U
51	1	2613	U
51	1	2615	U
51	1	2636	C
51	1	2646	C
51	1	2654	A
51	1	2689	U
51	1	2690	U
51	1	2714	G
51	1	2716	C
51	1	2720	U
51	1	2724	U
51	1	2733	A
51	1	2744	G
51	1	2748	A
51	1	2757	A
51	1	2758	A
51	1	2764	A
51	1	2765	A
51	1	2778	A
51	1	2779	U
51	1	2791	G
51	1	2793	C
51	1	2798	U
51	1	2800	A
51	1	2801	G
51	1	2820	A

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Mol	Chain	Res	Type
51	1	2821	A
51	1	2867	G
51	1	2868	A
51	1	2872	A
51	1	2880	C
51	1	2884	U
51	1	2893	A
52	2	2	G
52	2	4	C
52	2	13	G
52	2	35	C
52	2	53	A
52	2	56	G
52	2	67	G
52	2	88	C
52	2	89	U
52	2	90	C
52	2	108	A
52	2	109	A
53	3	6	G
53	3	9	G
53	3	22	G
53	3	32	A
53	3	39	G
53	3	44	A
53	3	48	C
53	3	50	A
53	3	51	A
53	3	54	C
53	3	71	A
53	3	78	A
53	3	84	U
53	3	85	U
53	3	87	C
53	3	92	U
53	3	94	G
53	3	100	G
53	3	101	A
53	3	110	C
53	3	121	U
53	3	130	A
53	3	144	G

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Mol	Chain	Res	Type
53	3	173	U
53	3	183	C
53	3	197	A
53	3	208	U
53	3	210	C
53	3	211	G
53	3	247	G
53	3	251	G
53	3	253	A
53	3	266	G
53	3	267	C
53	3	280	C
53	3	281	G
53	3	289	G
53	3	328	C
53	3	352	C
53	3	354	G
53	3	367	U
53	3	369	G
53	3	372	C
53	3	397	A
53	3	413	G
53	3	414	A
53	3	419	C
53	3	421	U
53	3	422	C
53	3	423	G
53	3	429	U
53	3	467	U
53	3	468	A
53	3	474	G
53	3	479	U
53	3	480	U
53	3	485	U
53	3	486	U
53	3	495	A
53	3	496	A
53	3	497	G
53	3	509	A
53	3	531	U
53	3	532	A
53	3	547	A

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Mol	Chain	Res	Type
53	3	559	A
53	3	561	U
53	3	566	G
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	596	A
53	3	633	G
53	3	653	U
53	3	665	A
53	3	671	G
53	3	686	U
53	3	687	A
53	3	688	G
53	3	703	G
53	3	724	G
53	3	731	G
53	3	733	G
53	3	755	G
53	3	777	A
53	3	793	U
53	3	794	A
53	3	814	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	821	G
53	3	842	U
53	3	843	U
53	3	844	G
53	3	846	G
53	3	887	G
53	3	902	G
53	3	934	C
53	3	935	A
53	3	938	A
53	3	943	U
53	3	960	U
53	3	963	G
53	3	966	G

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Mol	Chain	Res	Type
53	3	969	A
53	3	975	A
53	3	976	G
53	3	977	A
53	3	992	U
53	3	993	G
53	3	994	A
53	3	1004	A
53	3	1012	A
53	3	1026	G
53	3	1029	U
53	3	1031	C
53	3	1032	G
53	3	1033	G
53	3	1053	G
53	3	1054	C
53	3	1055	A
53	3	1086	U
53	3	1094	G
53	3	1096	C
53	3	1101	A
53	3	1130	A
53	3	1133	G
53	3	1136	C
53	3	1137	C
53	3	1138	G
53	3	1139	G
53	3	1146	A
53	3	1159	U
53	3	1168	U
53	3	1182	G
53	3	1184	G
53	3	1196	A
53	3	1212	U
53	3	1225	A
53	3	1238	A
53	3	1241	G
53	3	1275	A
53	3	1278	G
53	3	1280	A
53	3	1282	C
53	3	1286	U

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Mol	Chain	Res	Type
53	3	1287	A
53	3	1290	G
53	3	1299	A
53	3	1300	G
53	3	1301	U
53	3	1302	C
53	3	1305	G
53	3	1317	C
53	3	1320	C
53	3	1363	A
53	3	1378	C
53	3	1381	U
53	3	1394	A
53	3	1395	C
53	3	1398	A
53	3	1419	G
53	3	1422	G
53	3	1428	A
53	3	1431	A
53	3	1446	A
53	3	1448	C
53	3	1452	C
53	3	1453	G
53	3	1492	A
53	3	1497	G
53	3	1499	A
53	3	1503	A
53	3	1505	G
53	3	1506	U
53	3	1508	A
53	3	1517	G
53	3	1529	G
53	3	1530	G
54	4	4	U
54	4	8	U
62	5	2	C
62	5	7	A
62	5	8	U
62	5	9	A
62	5	11	C
62	5	13	C
62	5	15	G

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Mol	Chain	Res	Type
62	5	17	C
62	5	18	G
62	5	19	G
62	5	20	U
62	5	21	A
62	5	26	A
62	5	32	U
62	5	33	U
62	5	35	A
62	5	36	A
62	5	38	A
62	5	39	U
62	5	43	C
62	5	44	G
62	5	46	G
62	5	47	U
62	5	48	C
62	5	49	C
62	5	52	G
62	5	53	G
62	5	55	U
62	5	56	C
62	5	57	G
62	5	58	A
62	5	59	U
62	5	60	U
62	5	61	C
62	5	66	U
62	5	73	A
62	5	74	C
62	5	76	A
63	6	5	G
63	6	7	G
63	6	9	G
63	6	10	G
63	6	14	A
63	6	18	G
63	6	19	G
63	6	21	A
63	6	22	G
63	6	27	U
63	6	43	A

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Mol	Chain	Res	Type
63	6	44	A
63	6	45	G
63	6	47	U
63	6	48	C
63	6	49	G
63	6	59	A
63	6	70	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	1	227	A
51	1	490	C
51	1	784	G
51	1	859	G
51	1	1020	A
51	1	1130	U
51	1	2296	U
51	1	2326	C
51	1	2756	U
51	1	2873	A
52	2	88	C
53	3	70	U
53	3	413	G
53	3	1012	A
53	3	1054	C
53	3	1301	U
53	3	1395	C
62	5	7	A
62	5	35	A
62	5	48	C
62	5	57	G
62	5	60	U
62	5	73	A
62	5	75	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
66	5OH	h	6	66	8,12,13	0.79	0	3,16,18	1.49	1 (33%)
66	KBE	h	1	66	8,8,9	0.61	0	7,8,10	1.20	1 (14%)
66	UAL	h	5	66	7,8,9	2.29	3 (42%)	5,9,11	2.91	2 (40%)
66	DPP	h	2	66	3,5,6	0.57	0	1,5,7	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	5OH	h	6	66	-	0/2/18/20	0/1/1/1
66	KBE	h	1	66	-	0/7/7/8	-
66	UAL	h	5	66	-	0/3/7/9	-
66	DPP	h	2	66	-	0/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	h	5	UAL	C1-N1	-4.83	1.32	1.40
66	h	5	UAL	C-CA	-2.90	1.40	1.45
66	h	5	UAL	CA-N	2.02	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	h	5	UAL	CA-CB-N1	-5.29	115.63	125.60
66	h	5	UAL	O-C-CA	-3.24	121.27	125.39
66	h	6	5OH	CR-CB-CA	-2.33	110.09	112.61
66	h	1	KBE	CB-CA-C	-2.04	109.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	h	6	5OH	4	0
66	h	5	UAL	2	0
66	h	2	DPP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
68	GDP	0	801	-	24,30,30	0.93	1 (4%)	30,47,47	1.45	5 (16%)
69	PO4	0	802	-	4,4,4	1.11	0	6,6,6	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	GDP	0	801	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	0	801	GDP	C6-N1	-2.51	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	0	801	GDP	PA-O3A-PB	-4.36	117.86	132.83
68	0	801	GDP	C3'-C2'-C1'	2.55	104.82	100.98
68	0	801	GDP	C5-C6-N1	2.37	118.14	113.95
68	0	801	GDP	C8-N7-C5	2.24	107.25	102.99
68	0	801	GDP	O6-C6-C5	-2.09	120.29	124.37

There are no chirality outliers.

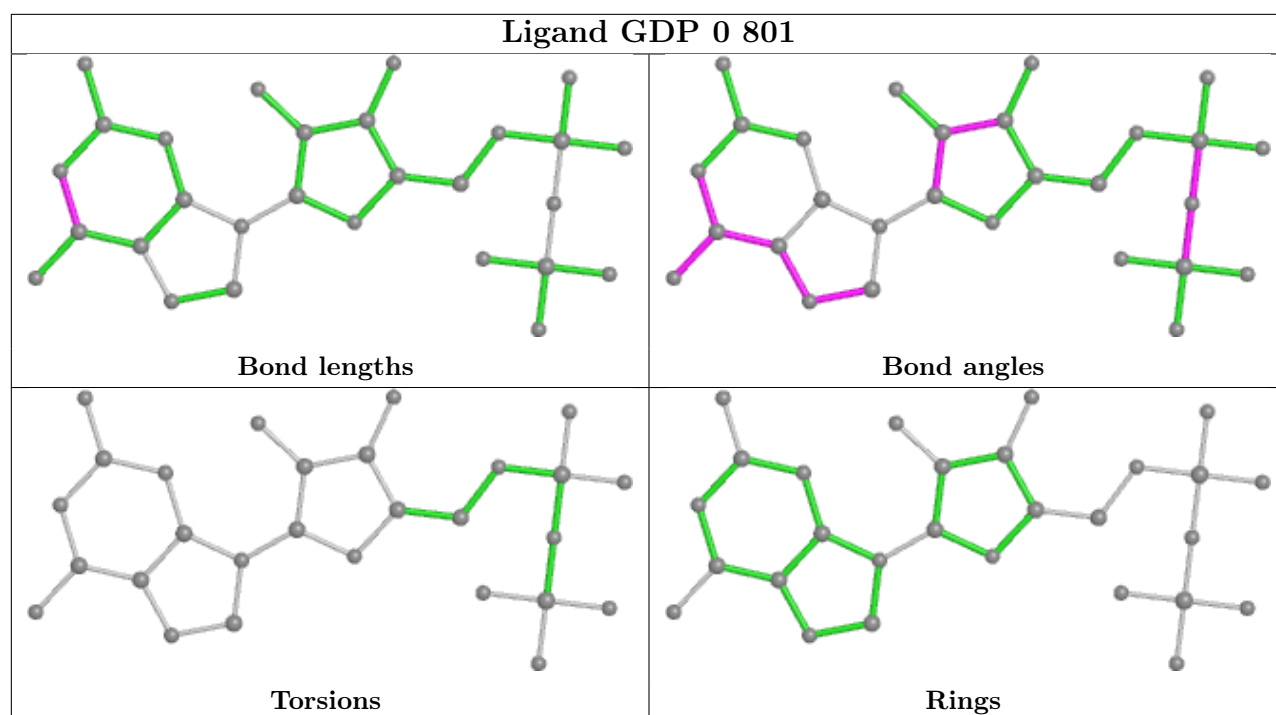
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	0	801	GDP	2	0
69	0	802	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

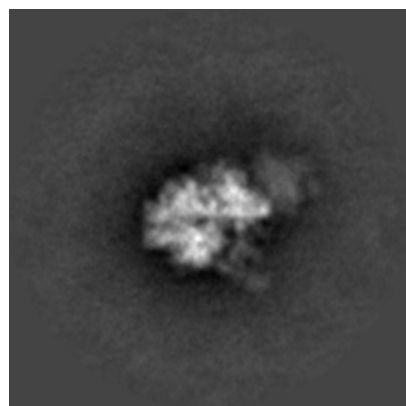
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38940. These allow visual inspection of the internal detail of the map and identification of artifacts.

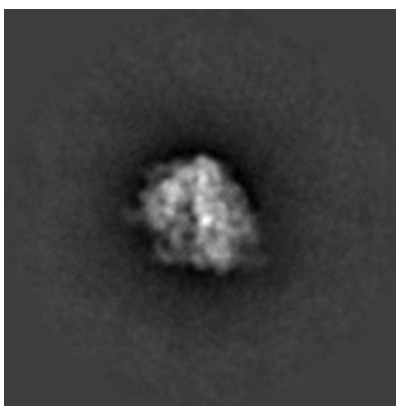
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

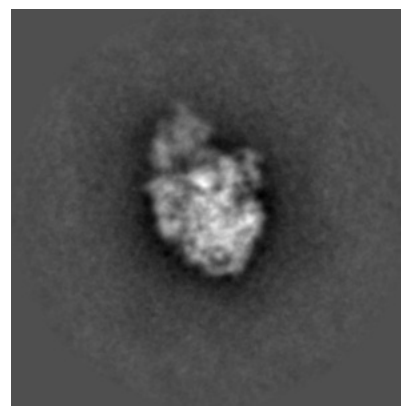
#### 6.1.1 Primary map



X

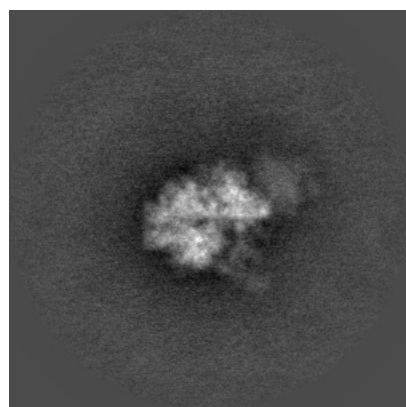


Y

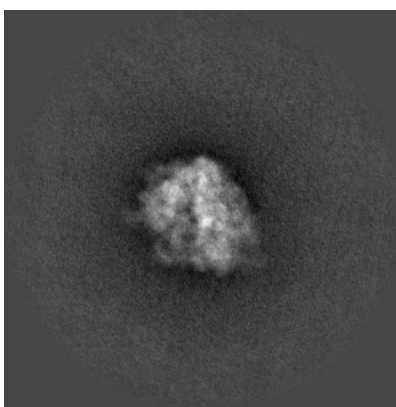


Z

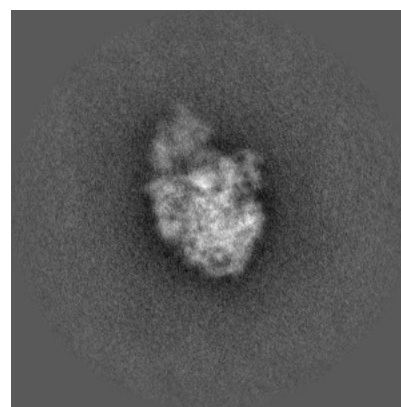
#### 6.1.2 Raw map



X



Y

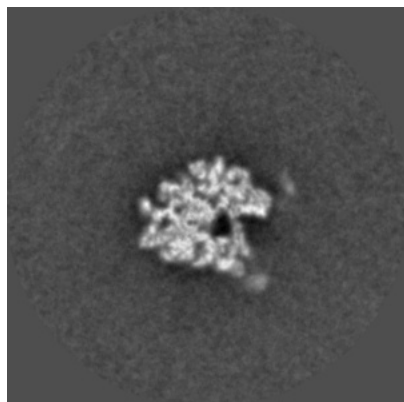


Z

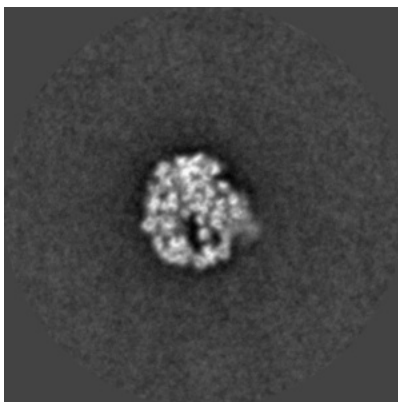
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

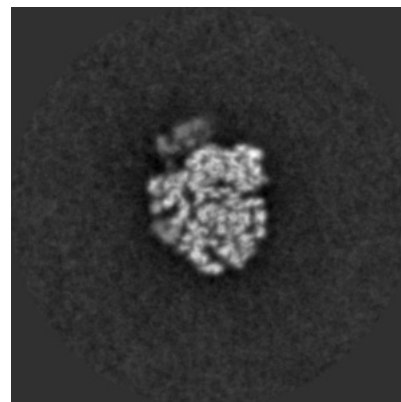
### 6.2.1 Primary map



X Index: 240

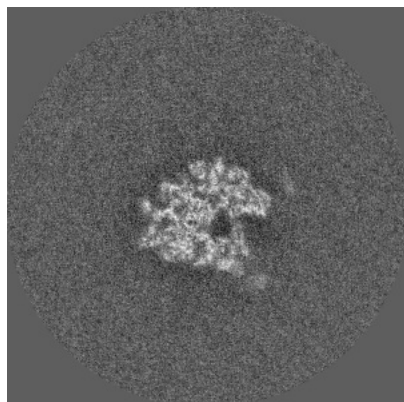


Y Index: 240

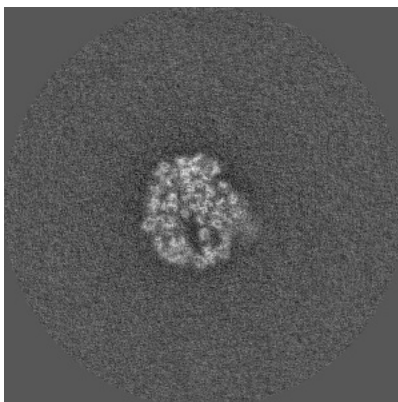


Z Index: 240

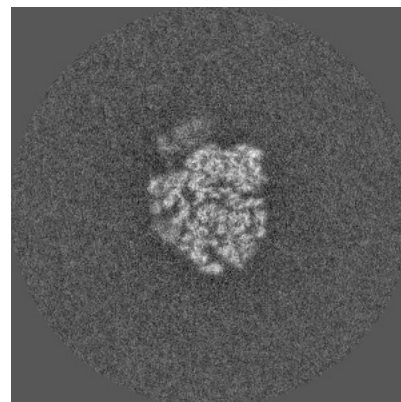
### 6.2.2 Raw map



X Index: 240



Y Index: 240



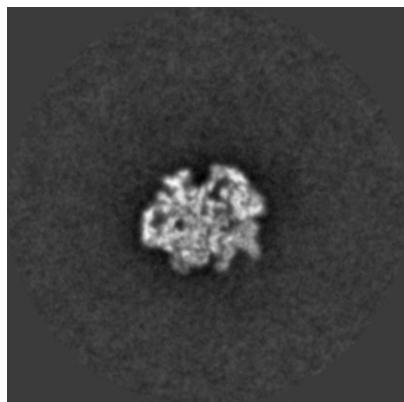
Z Index: 240

The images above show central slices of the map in three orthogonal directions.

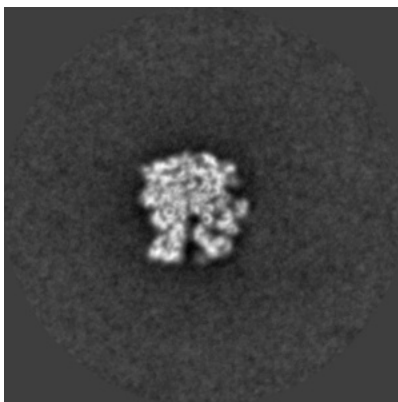


## 6.3 Largest variance slices [i](#)

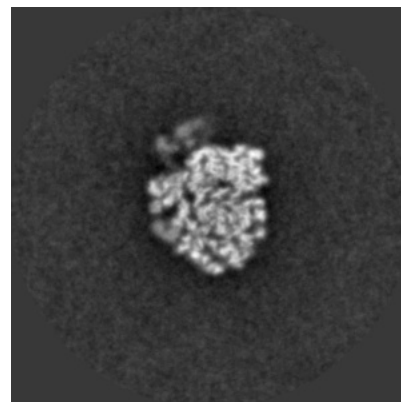
### 6.3.1 Primary map



X Index: 262

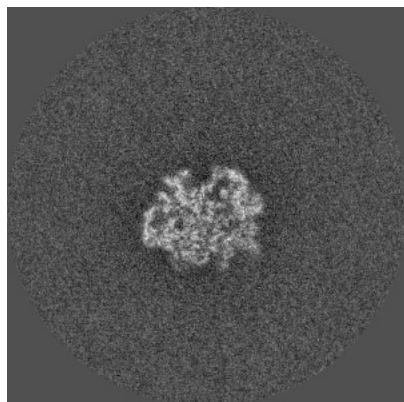


Y Index: 223

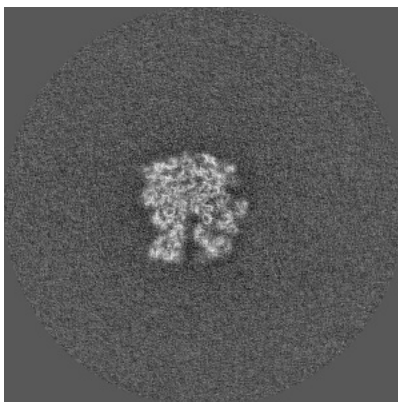


Z Index: 238

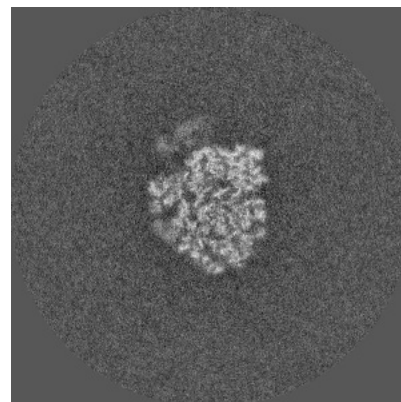
### 6.3.2 Raw map



X Index: 263



Y Index: 223

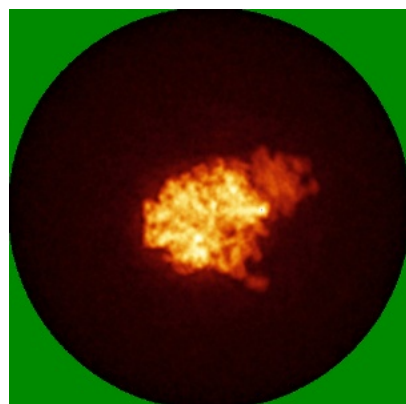


Z Index: 238

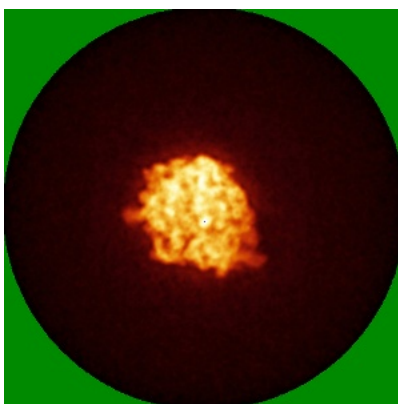
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

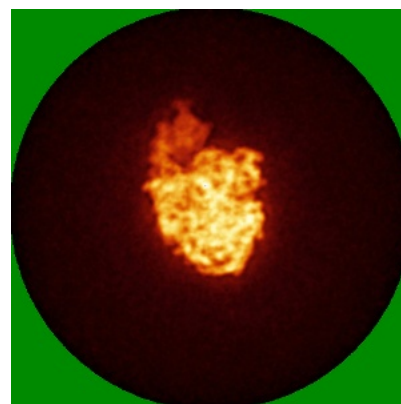
### 6.4.1 Primary map



X

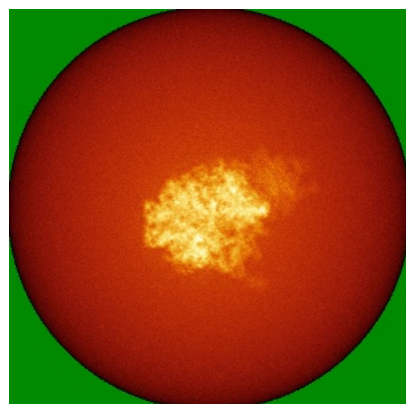


Y

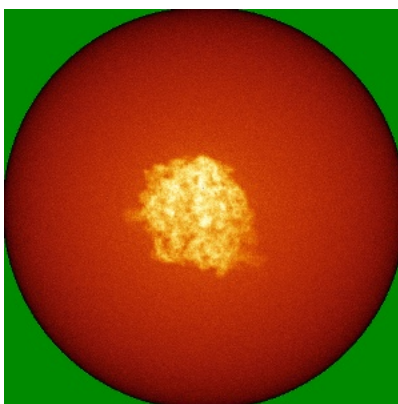


Z

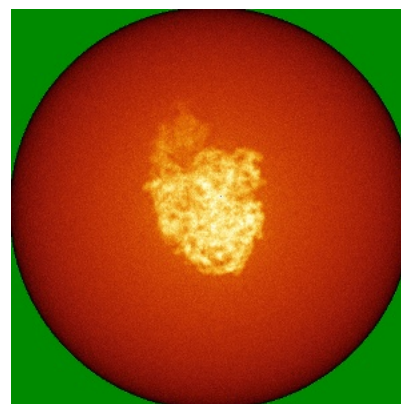
### 6.4.2 Raw map



X



Y

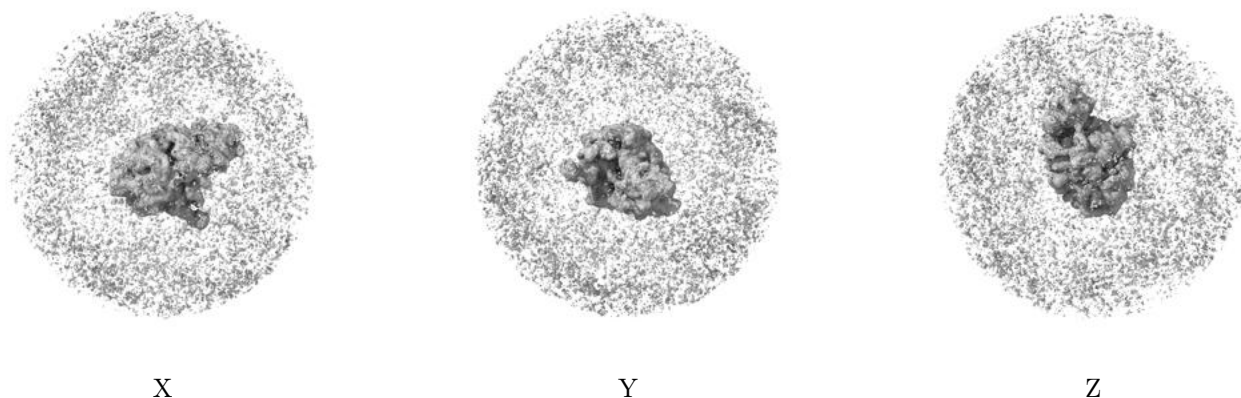


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

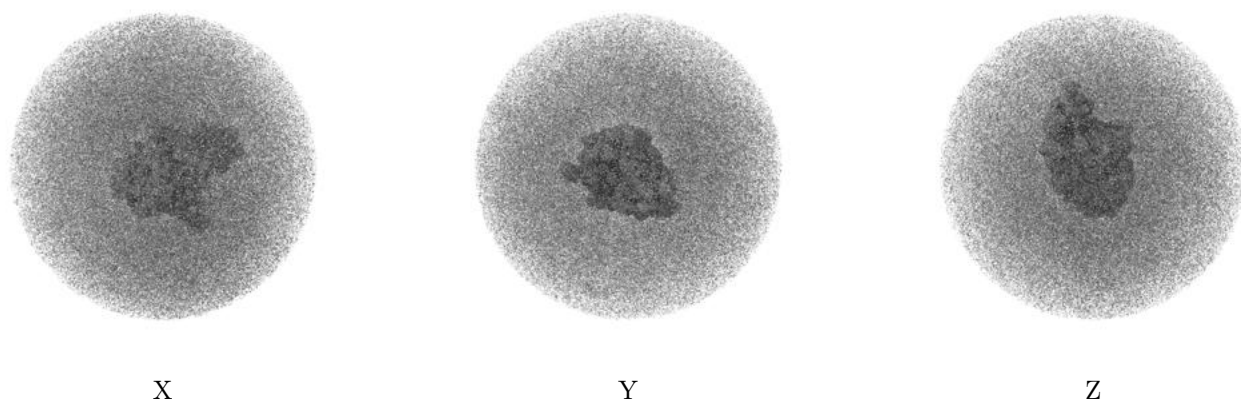
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

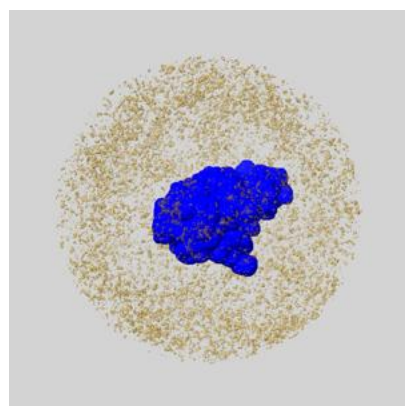
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

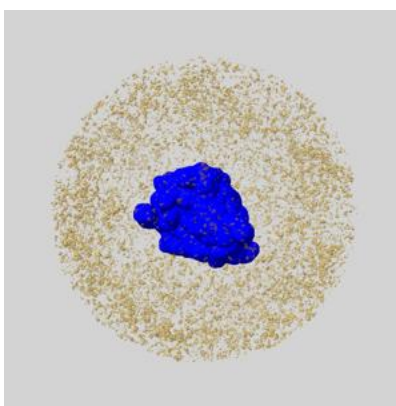
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

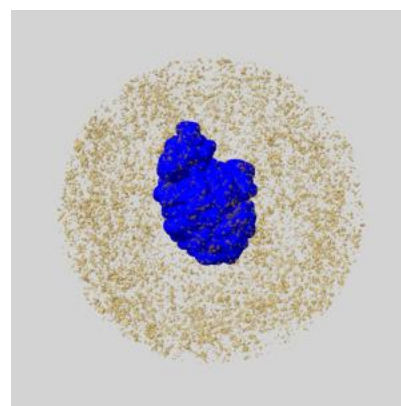
### 6.6.1 emd\_38940\_msk\_1.map [i](#)



X



Y

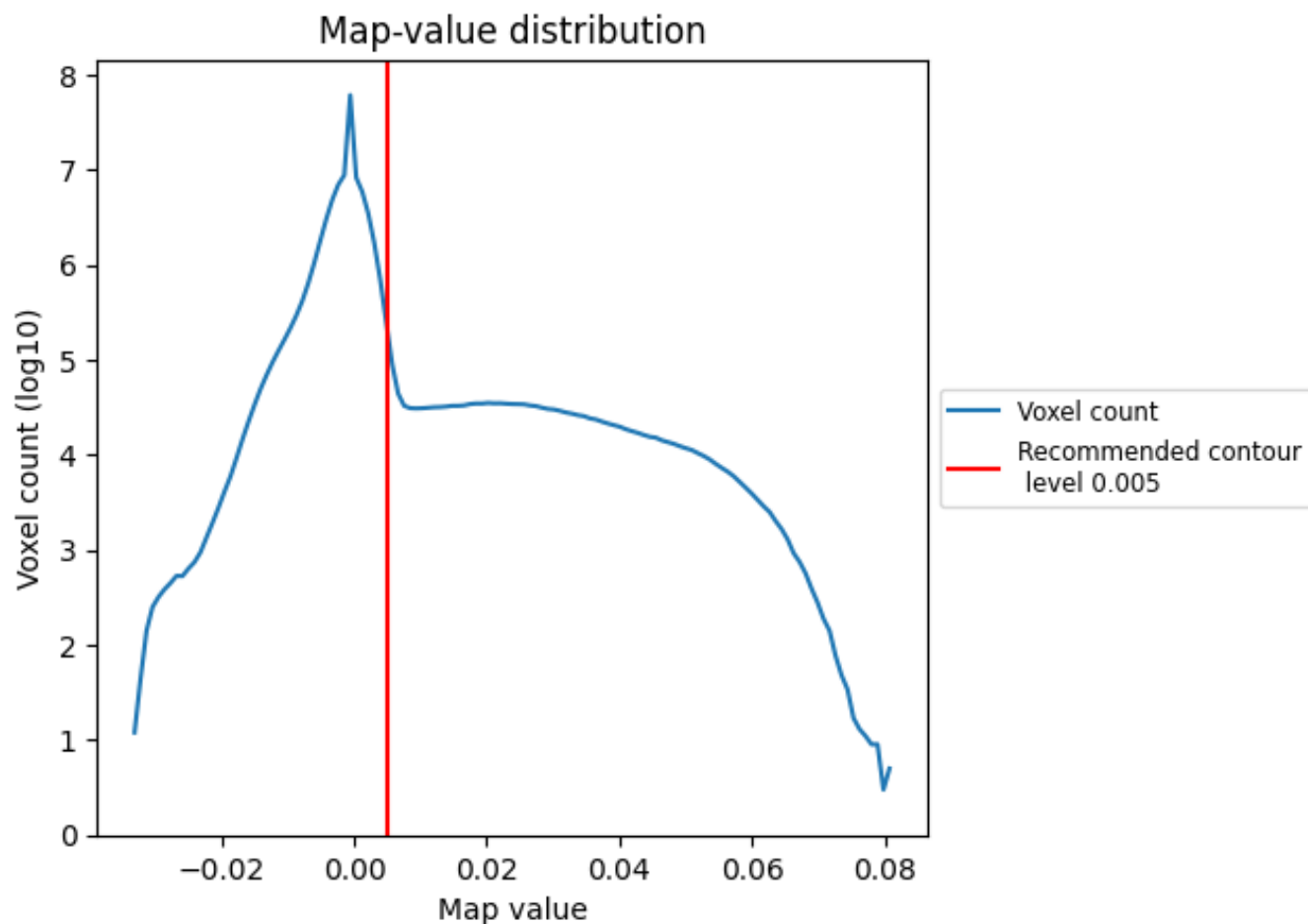


Z

## 7 Map analysis [i](#)

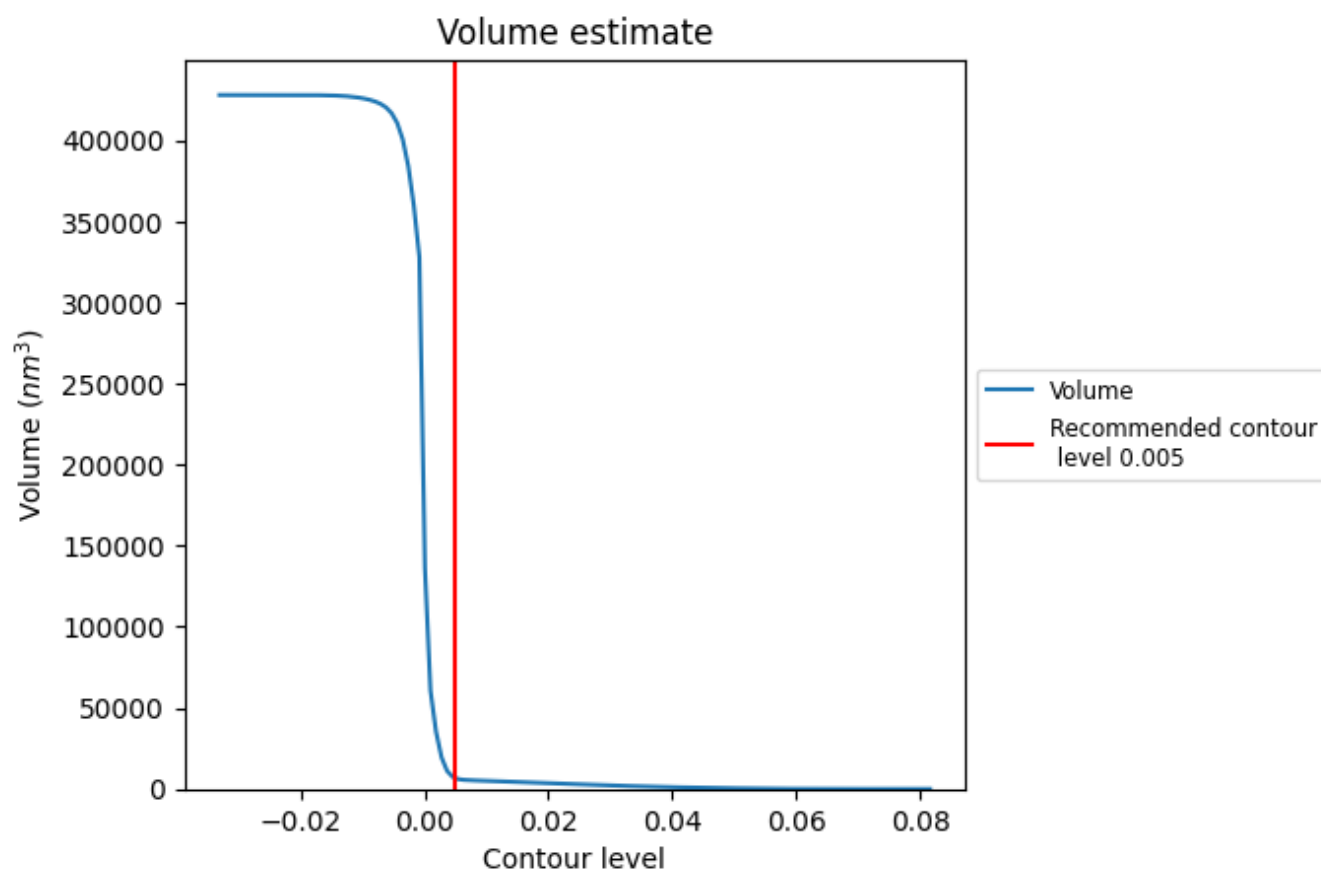
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

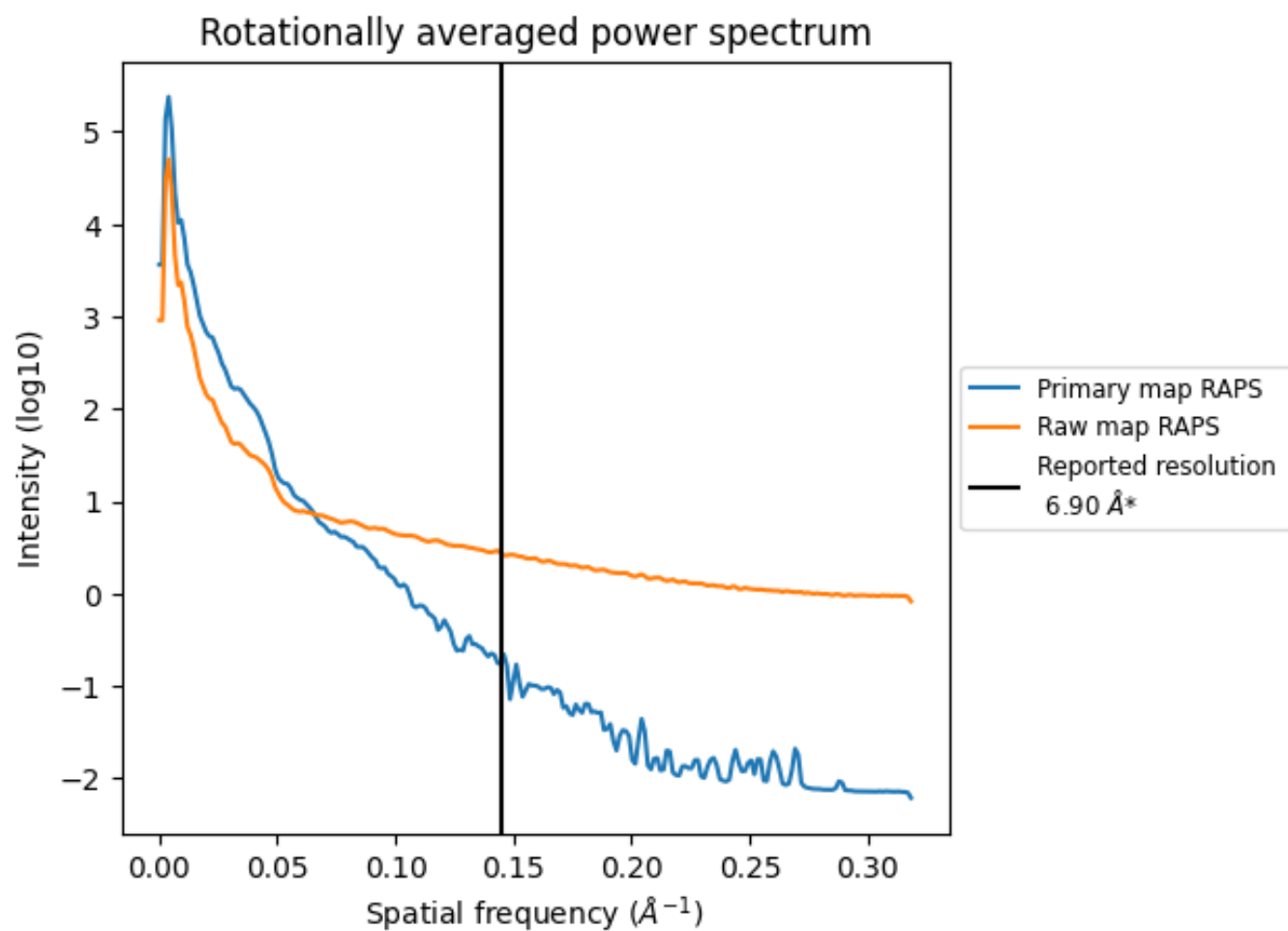


The volume at the recommended contour level is 6757  $\text{nm}^3$ ; this corresponds to an approximate mass of 6104 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

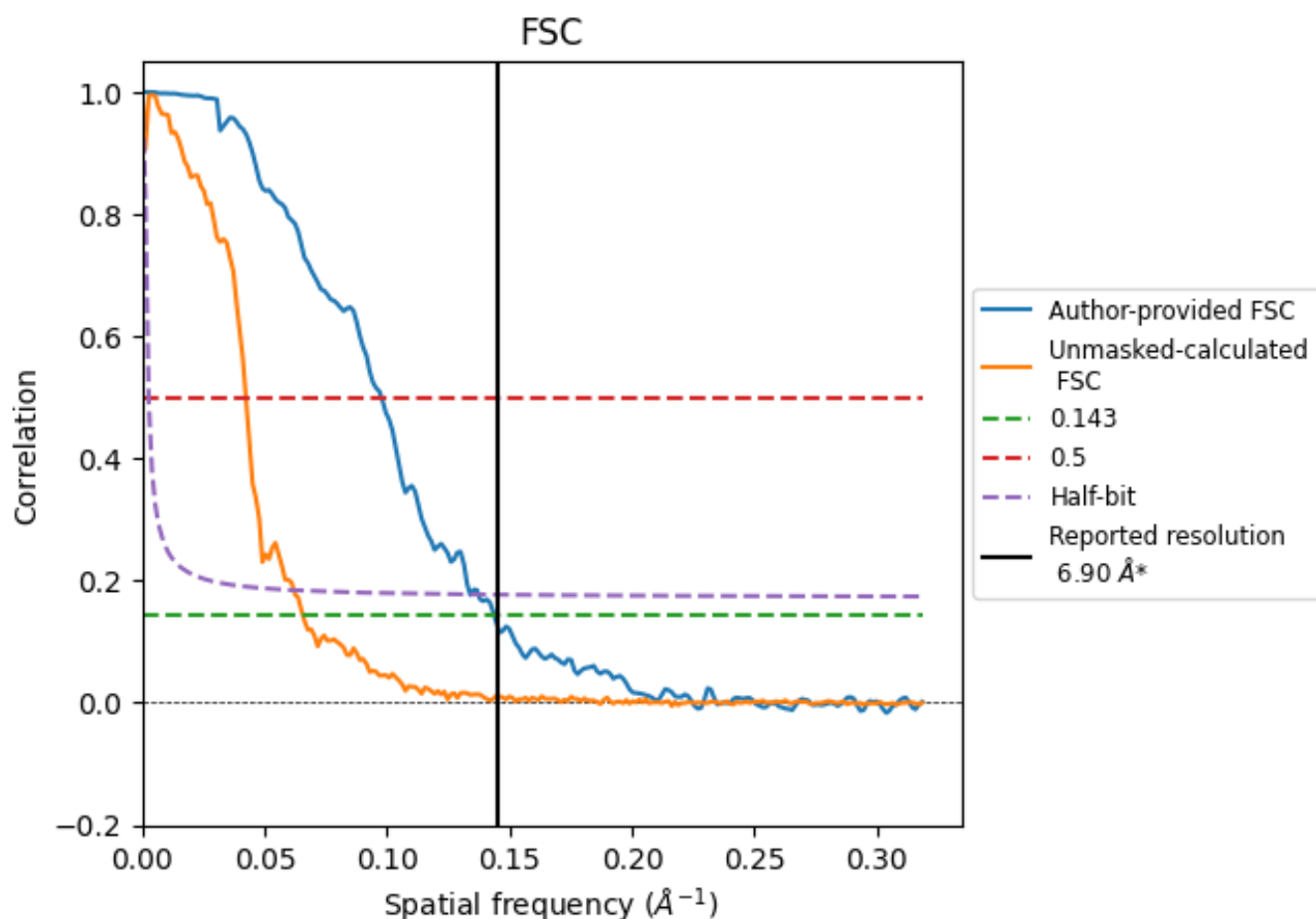


\*Reported resolution corresponds to spatial frequency of 0.145 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.145 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

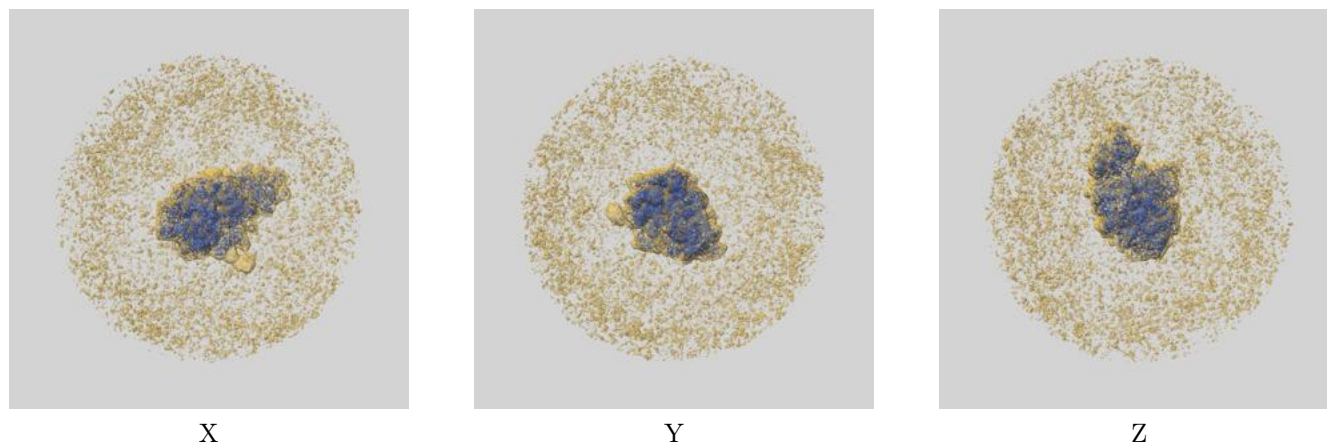
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	6.95	10.24	7.46
Unmasked-calculated*	15.22	23.64	16.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.22 differs from the reported value 6.9 by more than 10 %

## 9 Map-model fit [i](#)

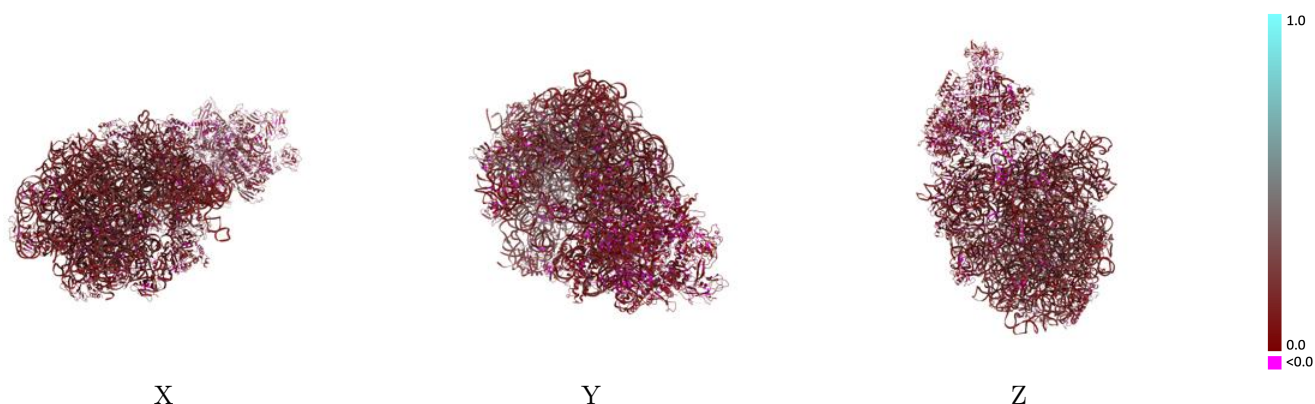
This section contains information regarding the fit between EMDB map EMD-38940 and PDB model 8Y5K. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

### 9.1 Map-model overlay [i](#)



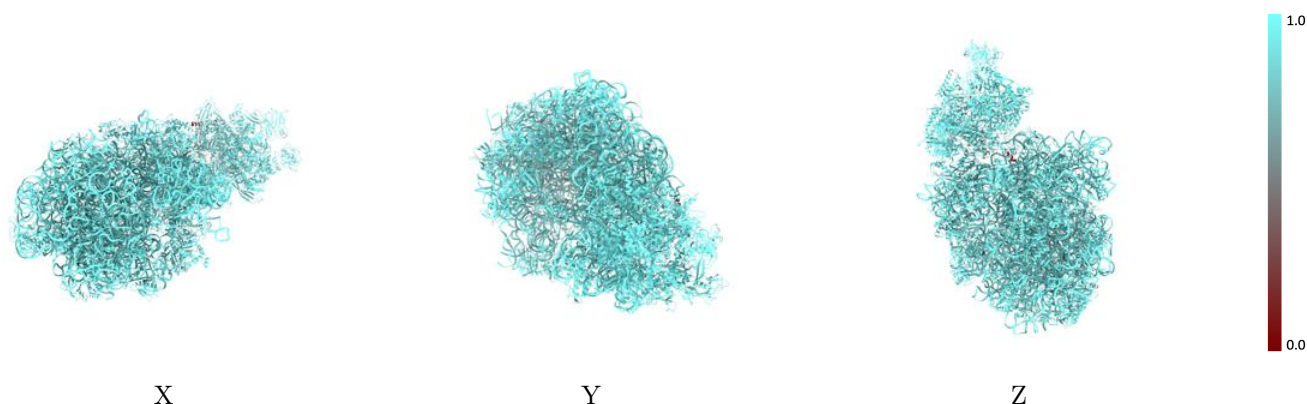
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



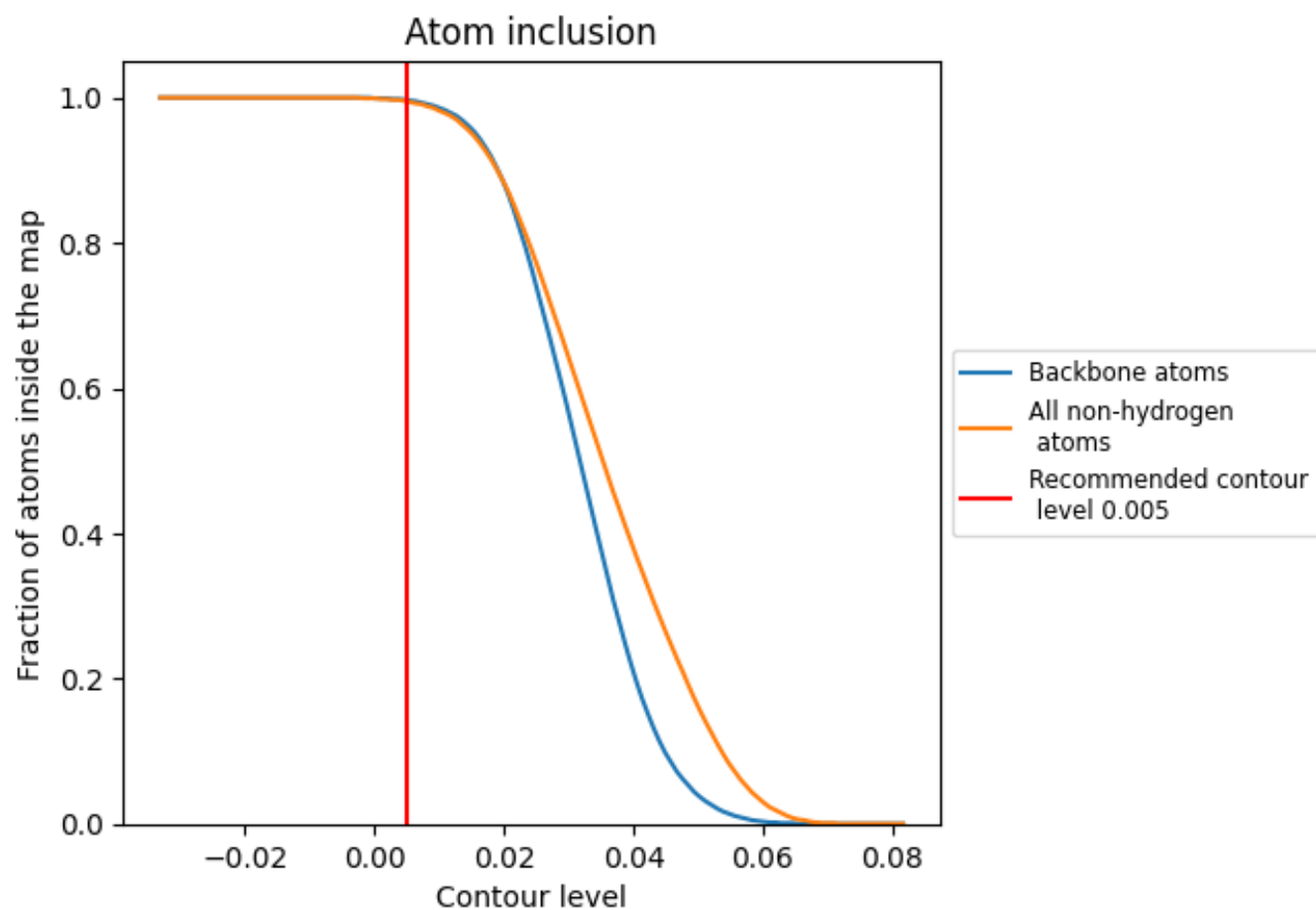
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



































































The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.1370
0	 0.9740	 0.1210
1	 1.0000	 0.1650
2	 1.0000	 0.1430
3	 1.0000	 0.1560
4	 1.0000	 0.1610
5	 0.9990	 0.1110
6	 0.9970	 0.1430
8	 1.0000	 0.1480
9	 1.0000	 0.1360
A	 0.9710	 0.0770
A1	 0.9900	 0.1070
A2	 0.9970	 0.1060
B	 1.0000	 0.0900
B1	 0.9880	 0.1060
B2	 0.9870	 0.0970
C	 0.9830	 0.0980
D	 0.9920	 0.0780
E	 1.0000	 0.0690
F	 1.0000	 0.0830
G	 0.9990	 0.1160
H	 0.9930	 0.1260
I	 0.9990	 0.1050
J	 0.9980	 0.1210
K	 0.9890	 0.1230
L	 0.9850	 0.1180
M	 0.9950	 0.1150
N	 0.9980	 0.0880
NG	 1.0000	 0.1490
O	 0.9990	 0.1010
P	 0.9990	 0.1250
Q	 0.9630	 0.1070
R	 0.9990	 0.1290
S	 1.0000	 0.0990
T	 0.9990	 0.1140



*Continued on next page...*

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Chain	Atom inclusion	Q-score
U	 1.0000	 0.1040
V	 0.9970	 0.1090
W	 1.0000	 0.1070
W0	 0.6910	 0.0270
X	 1.0000	 0.1030
Y	 0.9970	 0.1150
Z	 0.9850	 0.1060
a	 0.9930	 0.0730
b	 0.9940	 0.1240
c	 0.9940	 0.1070
d	 0.9970	 0.1100
e	 0.9790	 0.1070
f	 0.9960	 0.1110
g	 0.9390	 0.1060
h	 1.0000	 0.1450
i	 0.9920	 0.0860
j	 0.9990	 0.1100
k	 0.9890	 0.1430
l	 0.9980	 0.0860
m	 0.9960	 0.1220
n	 0.9990	 0.0980
o	 1.0000	 0.1050
p	 0.9890	 0.1370
q	 1.0000	 0.1070
r	 1.0000	 0.0990
s	 0.9990	 0.1160
t	 0.9960	 0.0920
u	 0.9990	 0.0980
v	 0.9990	 0.1030
w	 1.0000	 0.0880
x	 1.0000	 0.1150
y	 0.9980	 0.1170
z	 1.0000	 0.1140